Superconductivity and charge density wave physics near an antiferromagnetic quantum critical point: insights from Quantum Monte Carlo studies

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KITP Seminar 07/27/2017

Minnesota
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UNIVERSITY OF MINNESOTA
Driven to Discover℠

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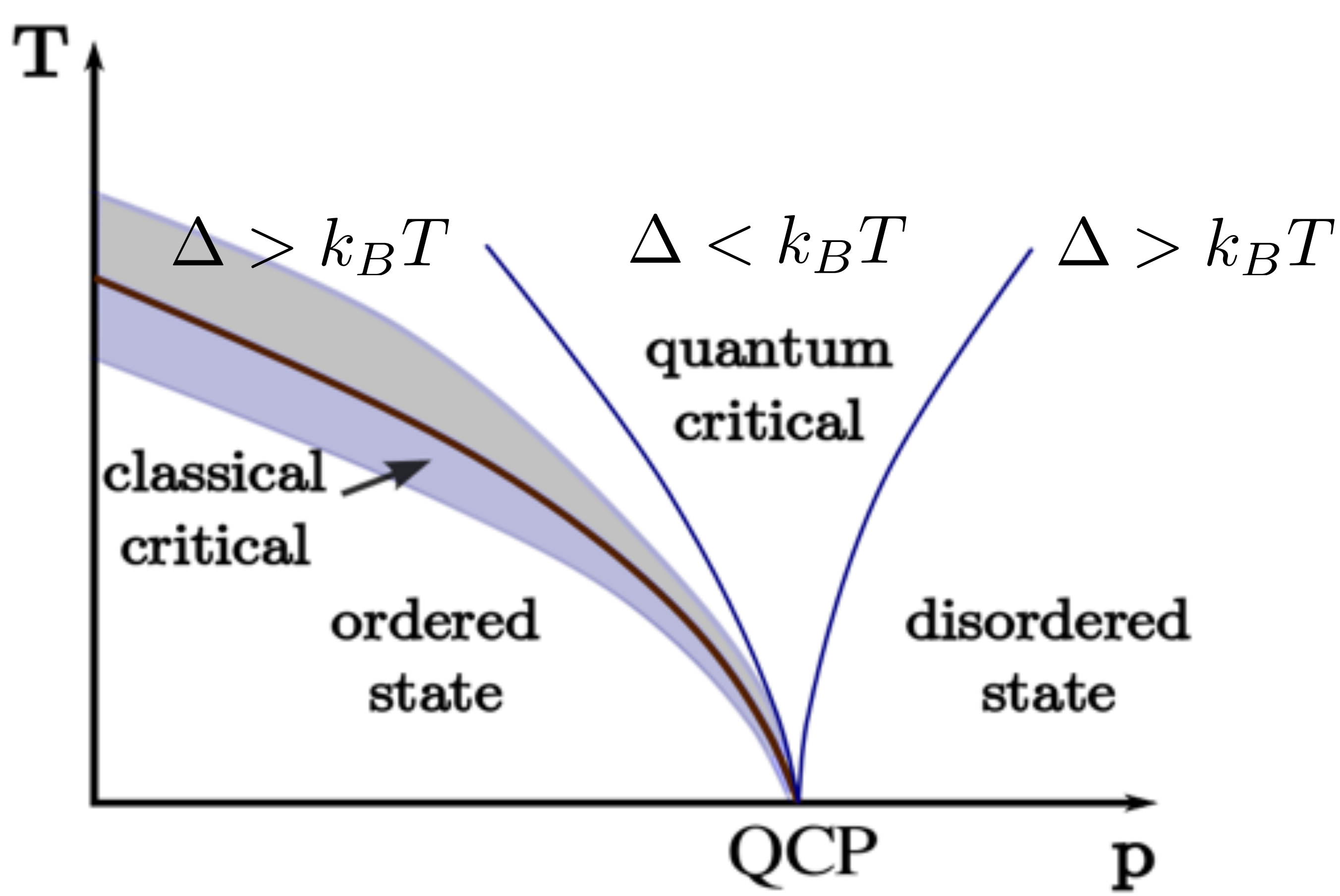
- Phys. Rev. B **95**, 174520 (2017)
- PR? (2017): in preparation

QCP as an organizing principle

- QCP: a continuous T=0 phase transition tuned by an external parameter
- QCPs well understood for insulators
  - e.g., transverse field Ising model
  - Quantum critical “fan” at finite T: temporal fluctuations are important
- What happens at a metallic QCP?
  - Non Fermi liquid behavior
  - Enhanced Tc for emergent electronic orders



Hertz, PRB 1976; Millis, PRB 1993
Sachdev, Quantum Phase Transitions, 2007
…

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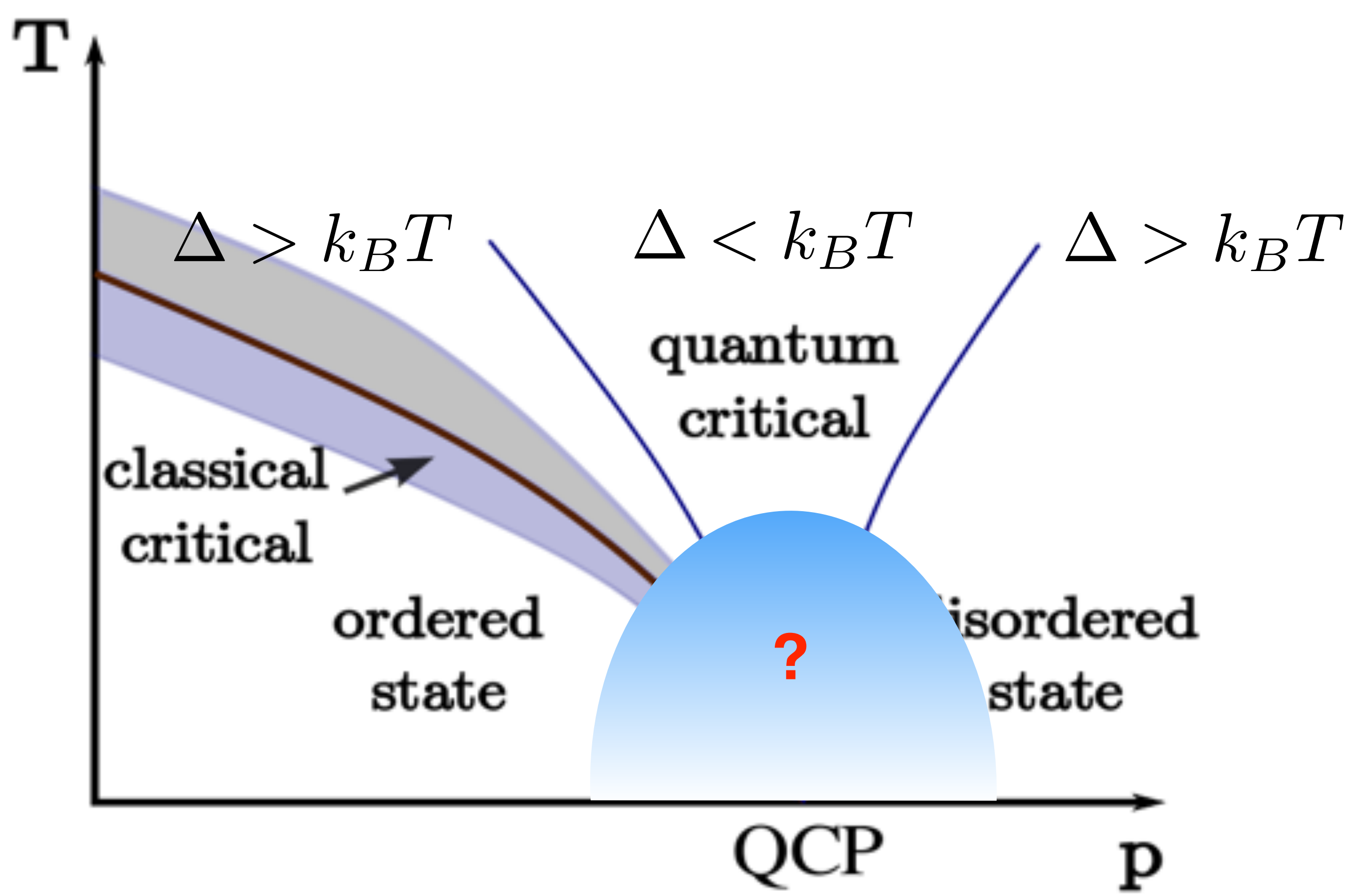

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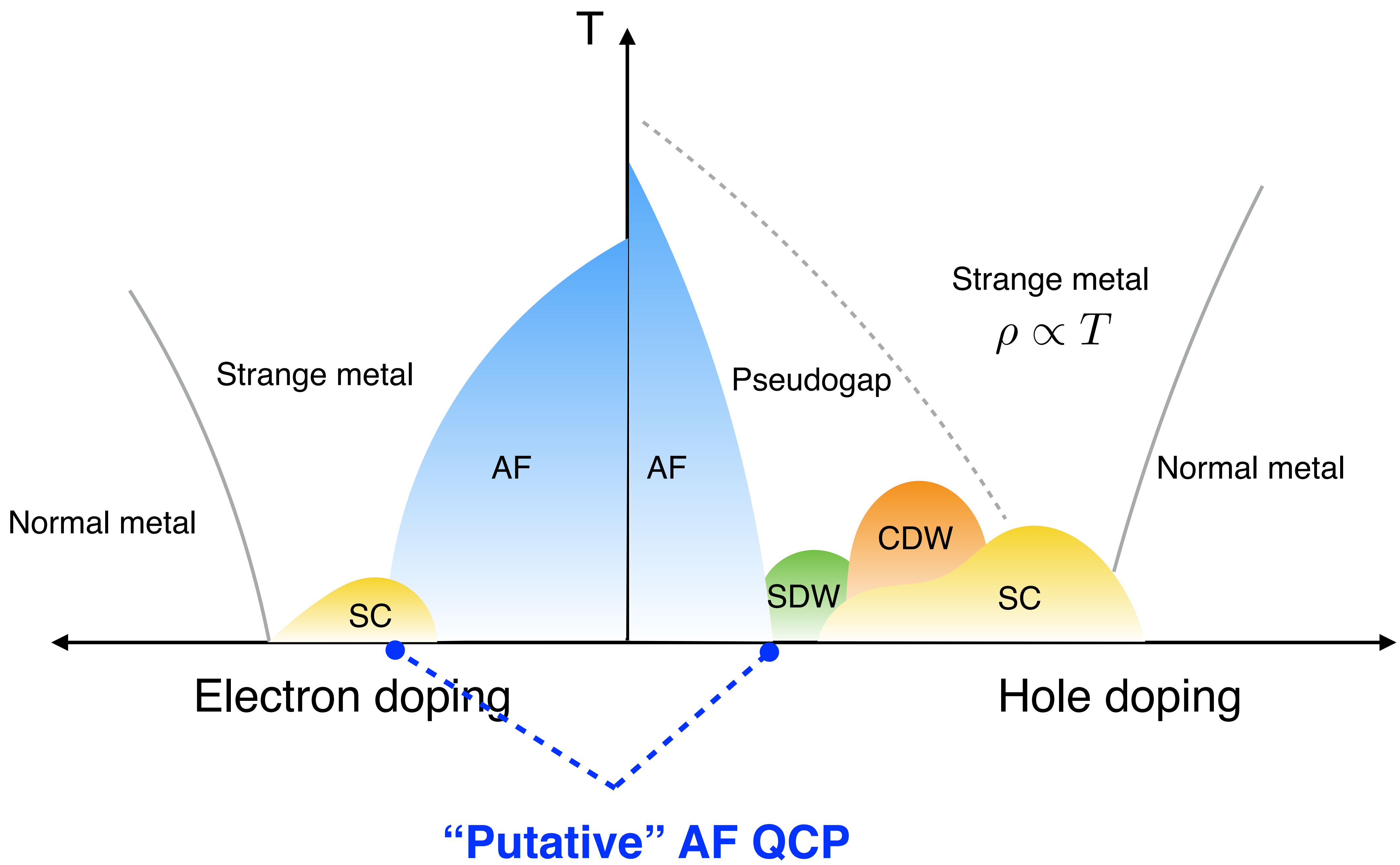
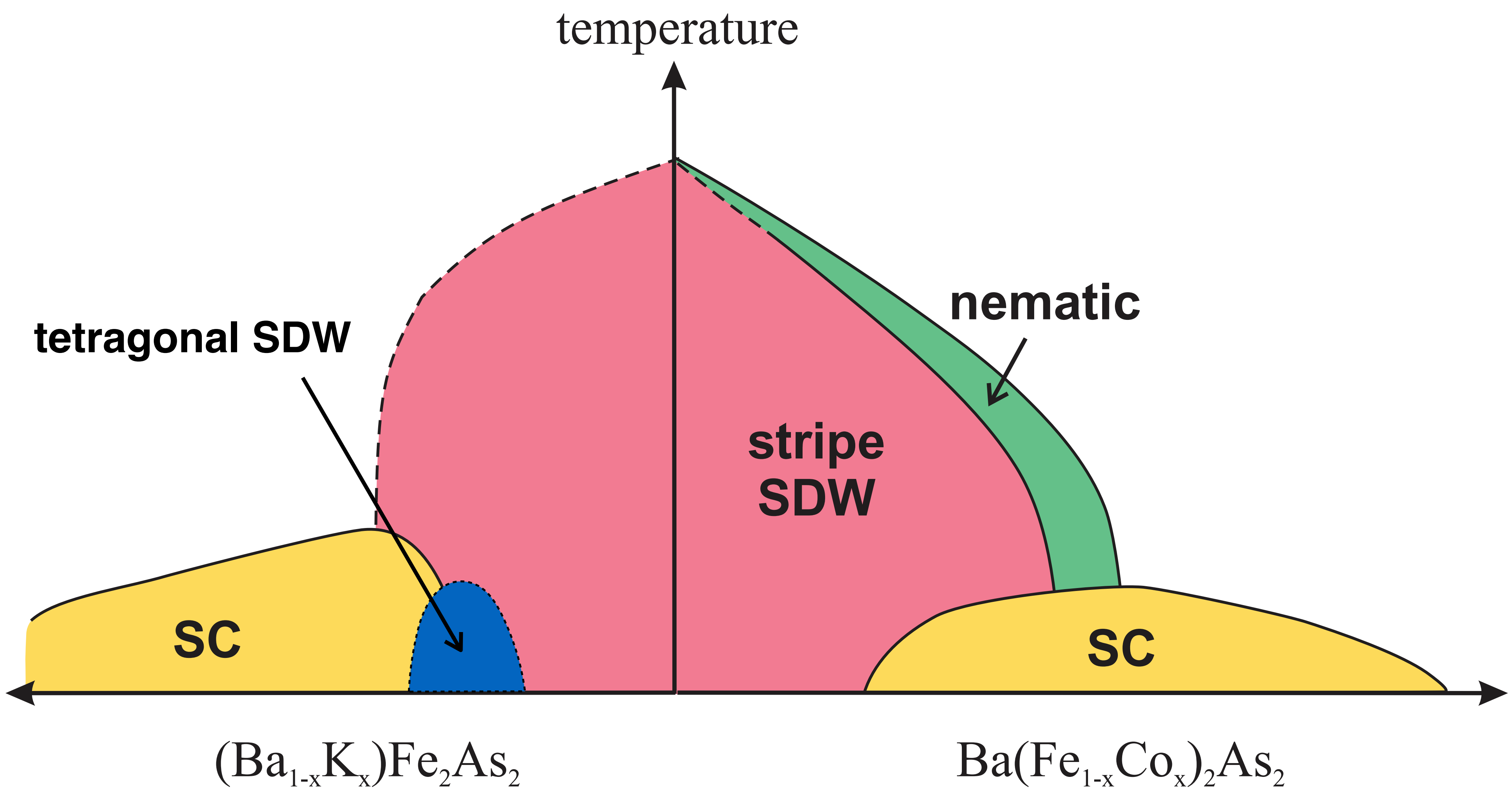
Cuprates



Adapted from Scalapino, RMP 2012

Iron pnictides



Adapted from Fernandes & Chubukov, Rep. Prog. Phys. (2017)

Contents

- Antiferromagnetic QCP and spin-fermion model
  - Hot spots and damped spin fluctuations
  - Emergent SU(2) and implications for SC and CDW
  - Eliashberg approximation
- What do we learn from numerics?
  - Sign-problem-free Quantum Monte Carlo
  - Superconductivity
  - CDW

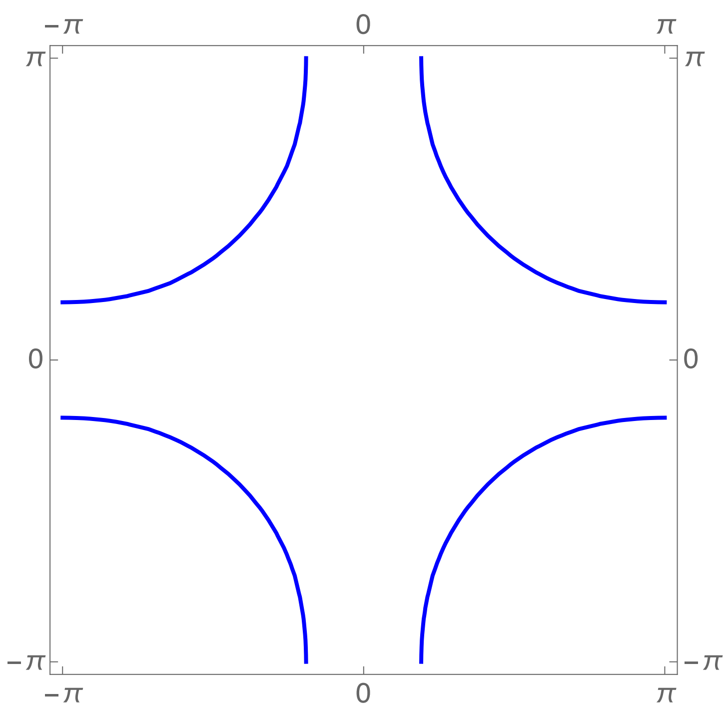
Spin-fermion model

Abanov, Chubukov & Schmalian, Adv. in Phys. (2003)
Metlitski & Sachdev, PRB (2010) …

- Effective low energy model
- Electrons near the Fermi surface coupled to quantum critical spin fluctuations

$$S_F = \int_\tau \sum_{\mathbf{k}\alpha} \bar{\psi}_{\mathbf{k}\alpha}(\partial_\tau + \varepsilon_{\mathbf{k}-\mu})\psi_{\mathbf{k}\alpha}$$

- Fermi surface



Spin-fermion coupling:

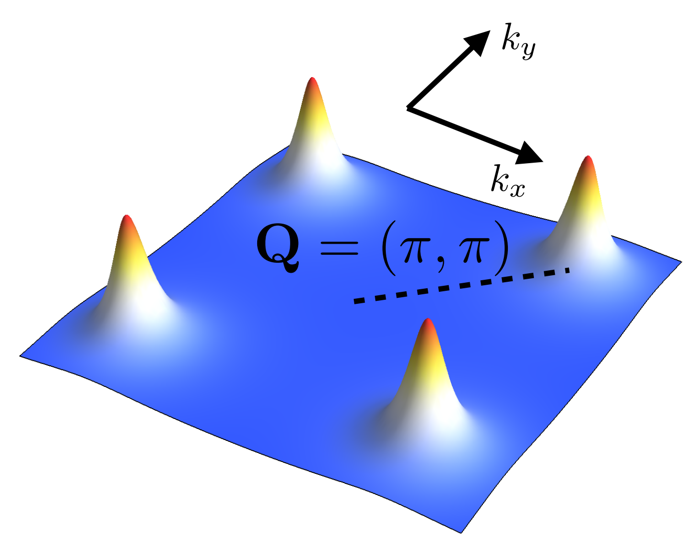
$$S_\lambda = \lambda \int_{\mathbf{x},\tau} \vec{\phi} \cdot \bar{\psi}_\alpha \vec{\sigma}_{\alpha\beta} \psi_\beta$$

$$S_B = \int_{\mathbf{q},i\Omega} \chi_0^{-1}(\mathbf{q}, i\Omega)\vec{\phi}_q \cdot \vec{\phi}_{-q}$$

- Magnetism comes from high energy
- Spin fluctuation peaked at **Q**

$$\chi_0^{-1}(\mathbf{q}, i\Omega) = r_0 + (\mathbf{q} - \mathbf{Q})^2 + \frac{\Omega^2}{v_s^2}$$

$r_0 > 0:$



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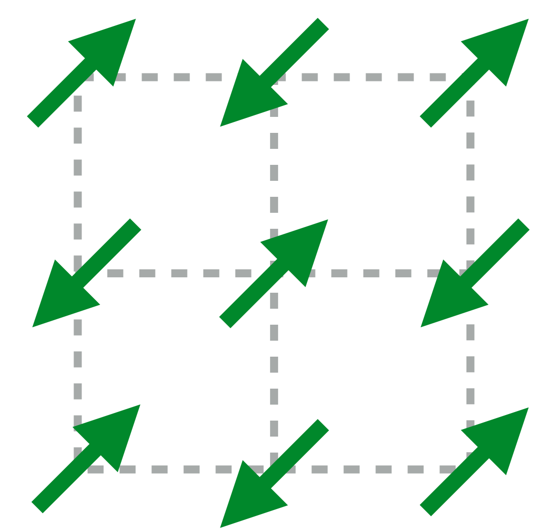


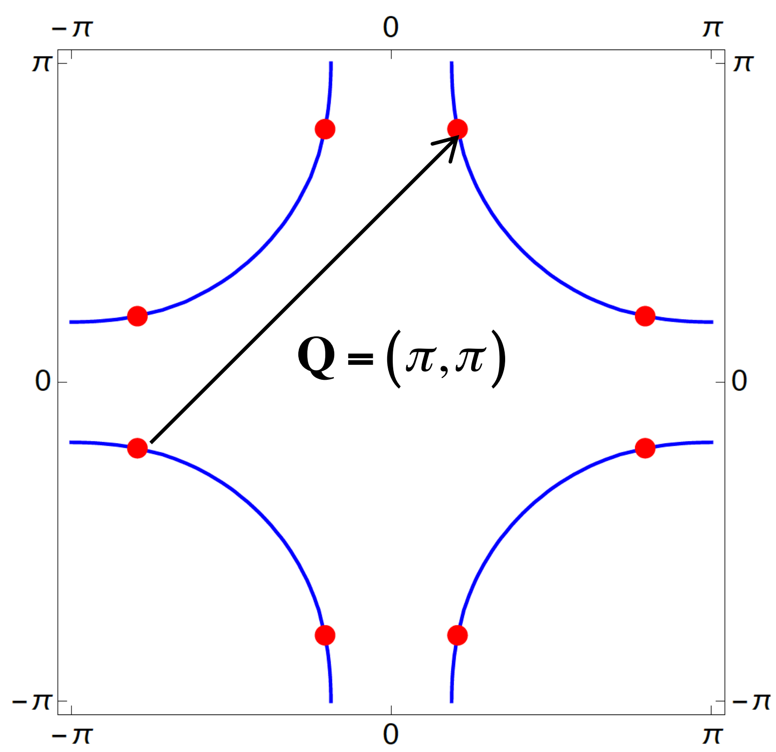
Néel order

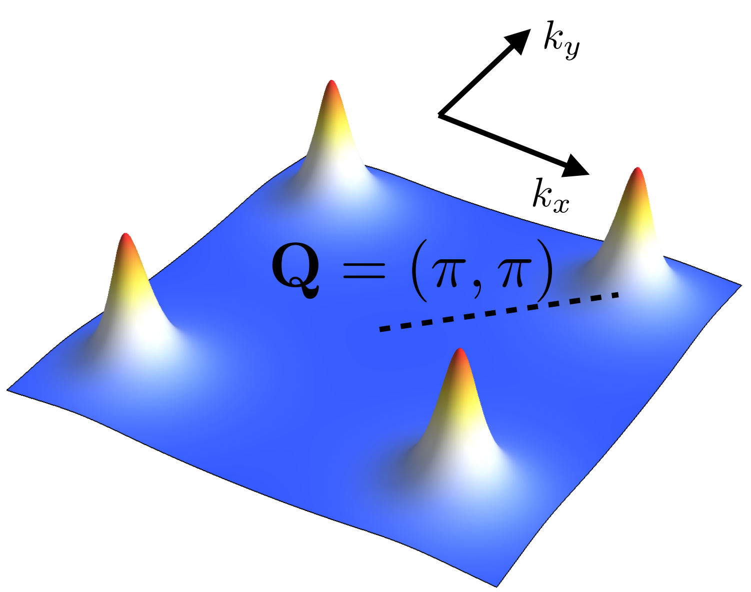
Analytical insights

Abanov, Chubukov & Schmalian, Adv. in Phys. (2003)
Metlitski & Sachdev, PRB (2010) …

Analytical insights

- Hot spots: Points on the Fermi surface that couple strongly to spin fluctuations





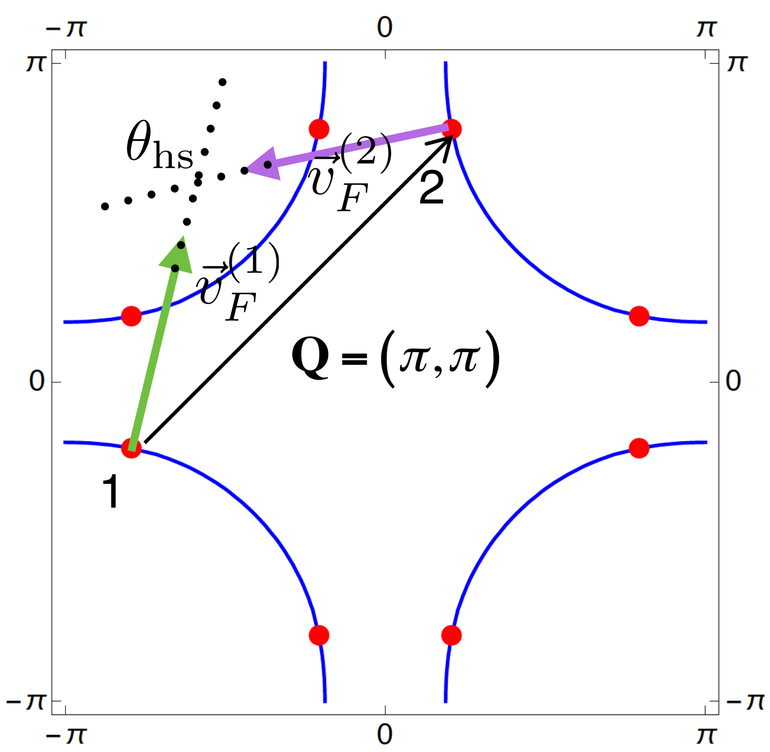
Abanov, Chubukov & Schmalian, Adv. in Phys. (2003)
Metlitski & Sachdev, PRB (2010) …

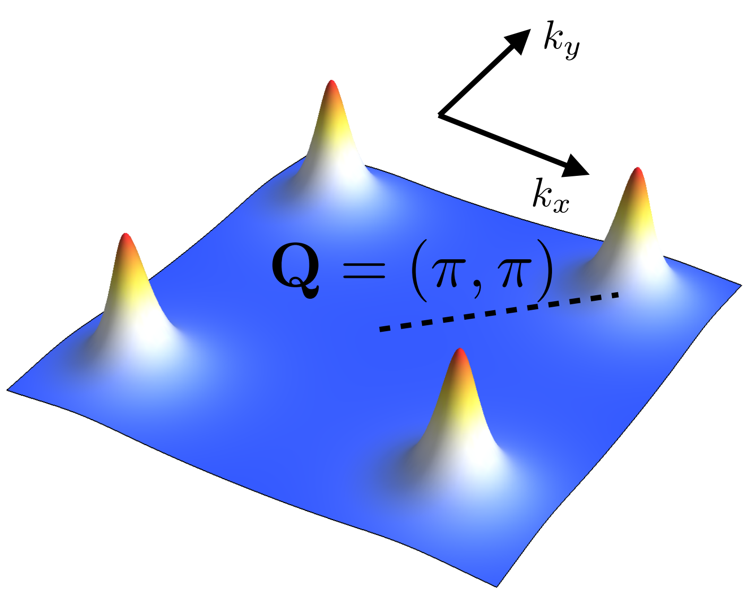
Analytical insights

- Hot spots: Points on the Fermi surface that couple strongly to spin fluctuations

- Low-energy physics governed by linearized hot spot approximation:

$$\varepsilon_{i,\mathbf{k}} \approx \mathbf{v}_F^{(i)} \cdot (\mathbf{k} - \mathbf{k}_{\rm hs}^{(i)});\ \ i = 1, 2$$





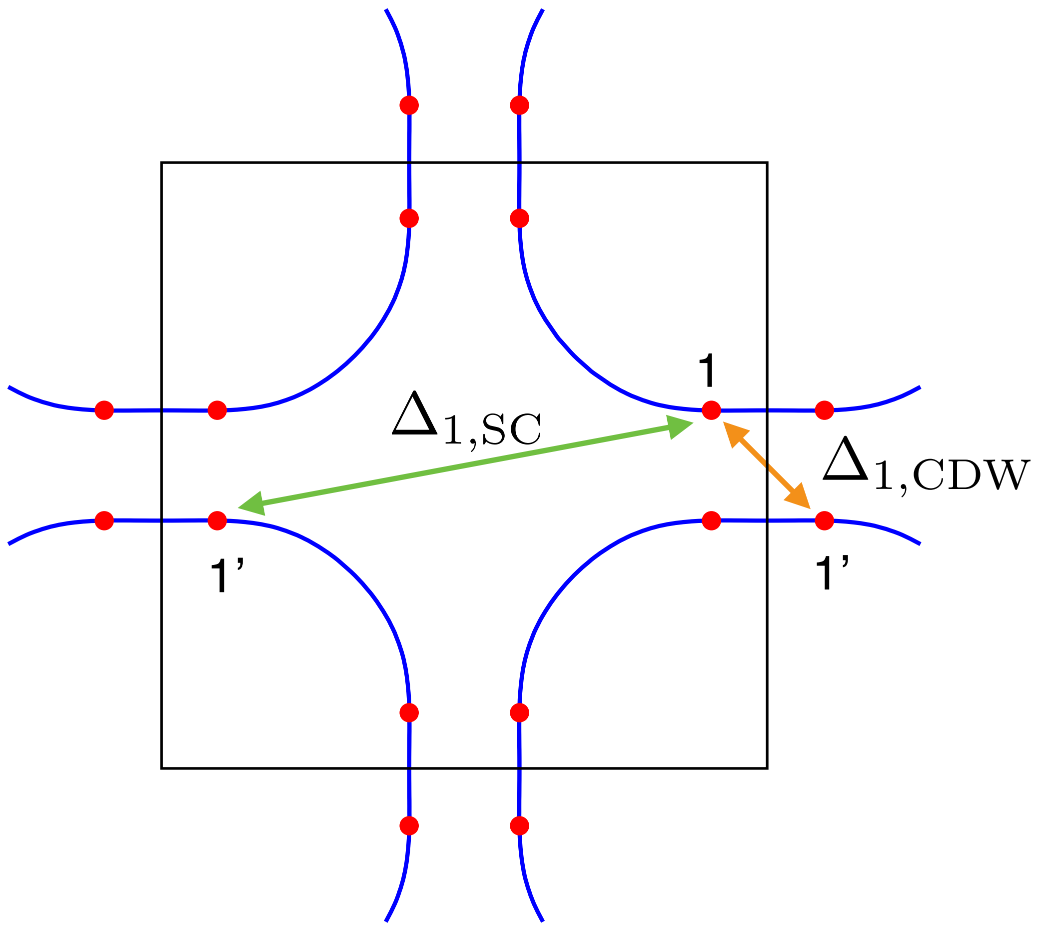
Abanov, Chubukov & Schmalian, Adv. in Phys. (2003)
Metlitski & Sachdev, PRB (2010) …

Analytical insights

- Emergent SU(2) symmetry at each pair of hot spots

$$\begin{pmatrix} \psi_{i,\mathbf{k}\uparrow} \\ \psi_{i,\mathbf{k}\downarrow} \end{pmatrix} \to \begin{pmatrix} \psi^\dagger_{i,-\mathbf{k}\downarrow} \\ -\psi^\dagger_{i,-\mathbf{k}\uparrow} \end{pmatrix} ;\ i = 1, 2$$

- Enlarged order parameter O(4): complex SC and CDW
    - Robust against perturbations?



$$\Delta_{1,\mathrm{SC}} = \langle \psi_{1,\uparrow}\psi_{1',\downarrow} - \psi_{1,\downarrow}\psi_{1',\uparrow} \rangle$$

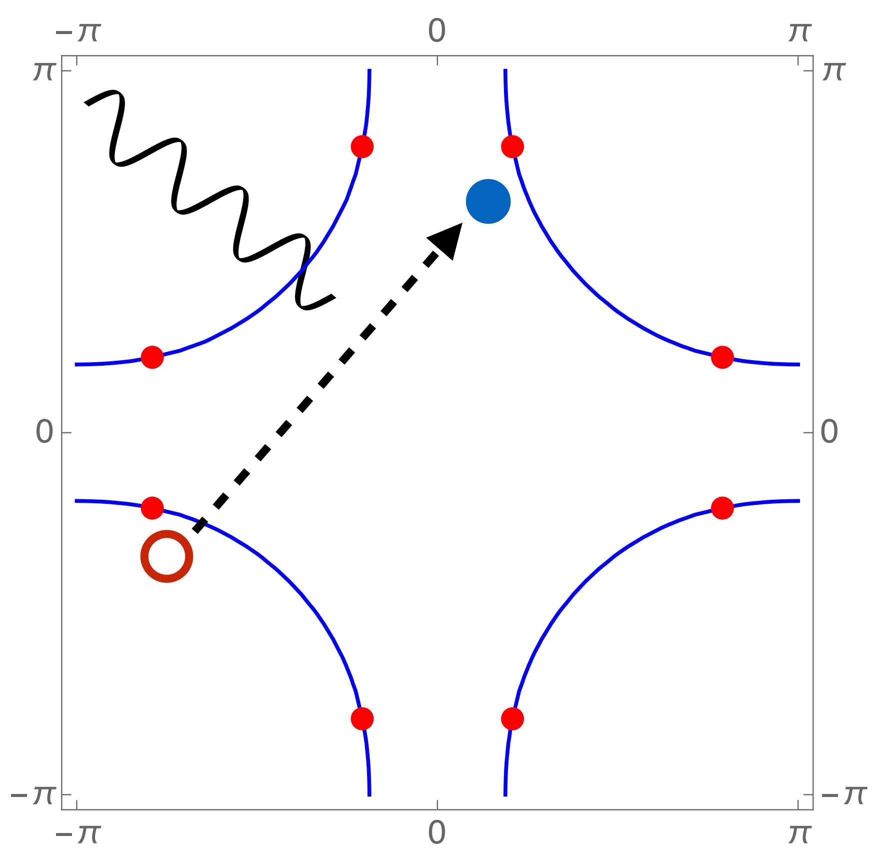
$$\Delta_{1,\mathrm{CDW}} = \langle \psi_{1,\uparrow}\psi^\dagger_{1',\uparrow} + \psi_{1,\downarrow}\psi^\dagger_{1',\downarrow} \rangle$$

Metlitski & Sachdev, PRB (2010)
Wang, Agterberg & Chubukov, PRB (2015)

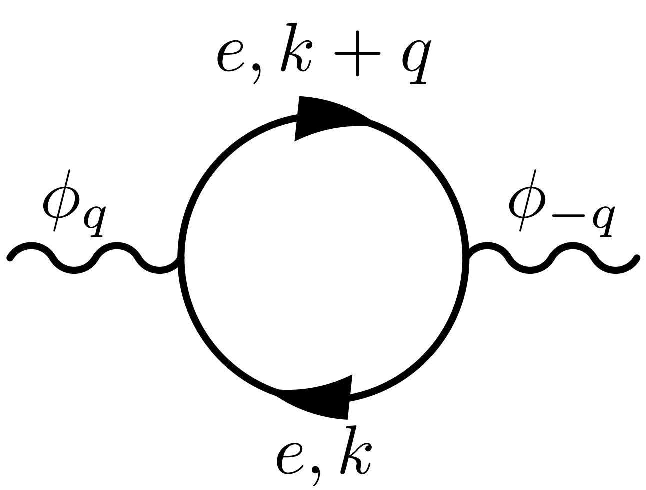
Analytical insights

- Spin fluctuations decay into an electron-hole pair near the Fermi surface
- Low frequency spin fluctuations are Landau-damped:

$$\chi(\mathbf{q}, i\Omega_n) = \frac{1}{r_0 + (\mathbf{q}-\mathbf{Q})^2 + \Omega_n^2/v_s^2 + \boxed{|\Omega_n|/\gamma}} \qquad \frac{1}{\gamma} \propto \frac{\lambda^2}{v_f^2 \sin(\theta_{\mathrm{hs}})}$$



Polarization bubble:



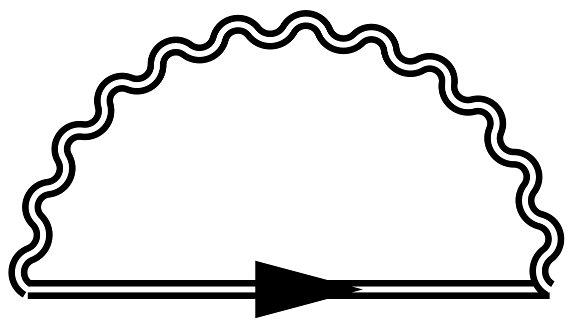
Abanov, Chubukov & Schmalian, Adv. in Phys. (2003)
Metlitski & Sachdev, PRB (2010)
Mross et al, PRB (2010) …

Analytical insights

- How to study SC and non-FL due to quantum critical spin fluctuations?

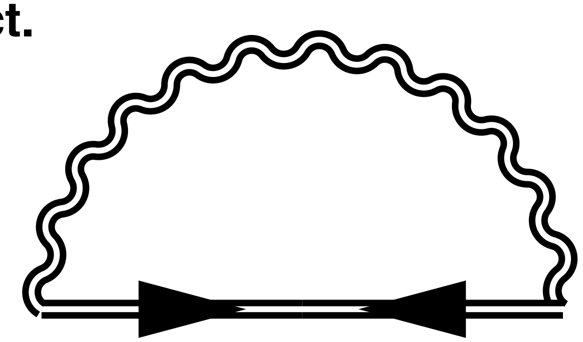
  —Hot-spot Eliashberg approximation

damped spin fluct.



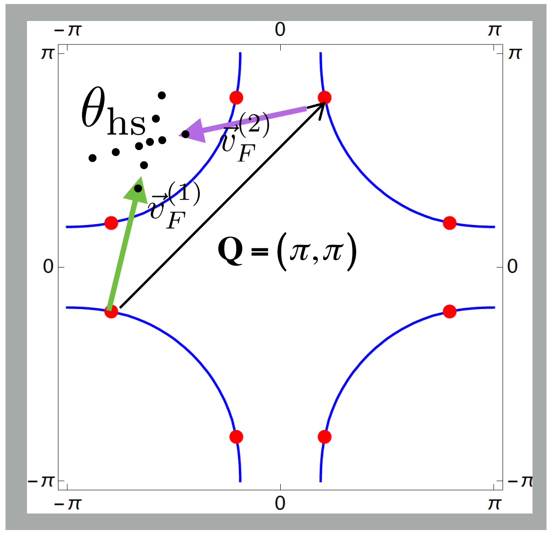
Regular part of the self-energy

$$\Sigma(\omega) \sim \sqrt{\omega}$$



Anomalous part of the self-energy

$$T_c \propto \left(\frac{\lambda^2}{v_F}\right)^2 \gamma \sim \lambda^2 \sin(\theta_{\rm hs})$$



- How to understand the angle dependence of T_c?
  - $\theta_{\rm hs} \to 0$: Spin fluct. strongly damped; insufficient to mediate pairing

Abanov, Chubukov & Schmalian, Adv. in Phys. (2003)
Metlitski & Sachdev, PRB (2010) …

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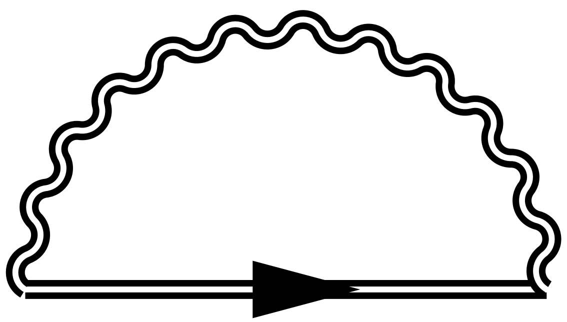

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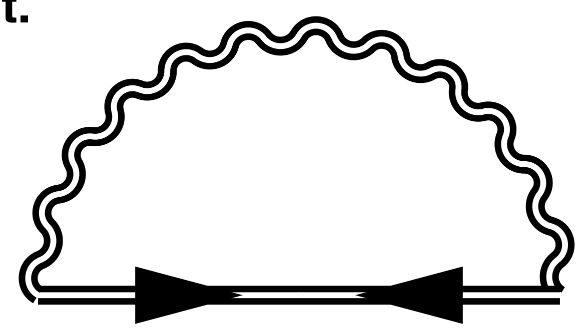

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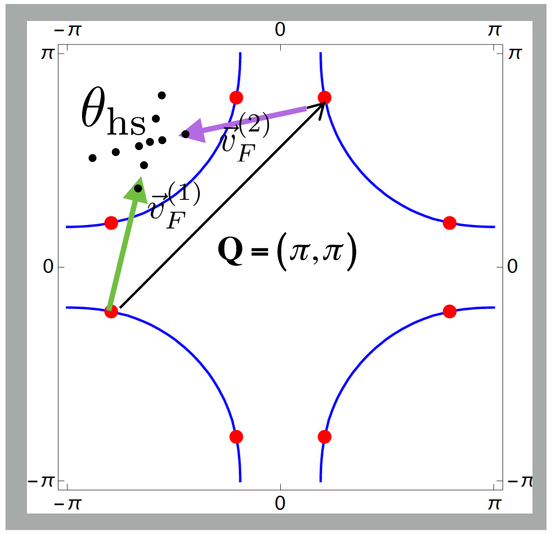


- How to understand the angle dependence of T_c?
  - $\theta_{\mathrm{hs}} \to 0$: Spin fluct. strongly damped; insufficient to mediate pairing

Assumpt. of hot-spot Eliashberg approx.:
Neglecting vertex correction; not fully justified!

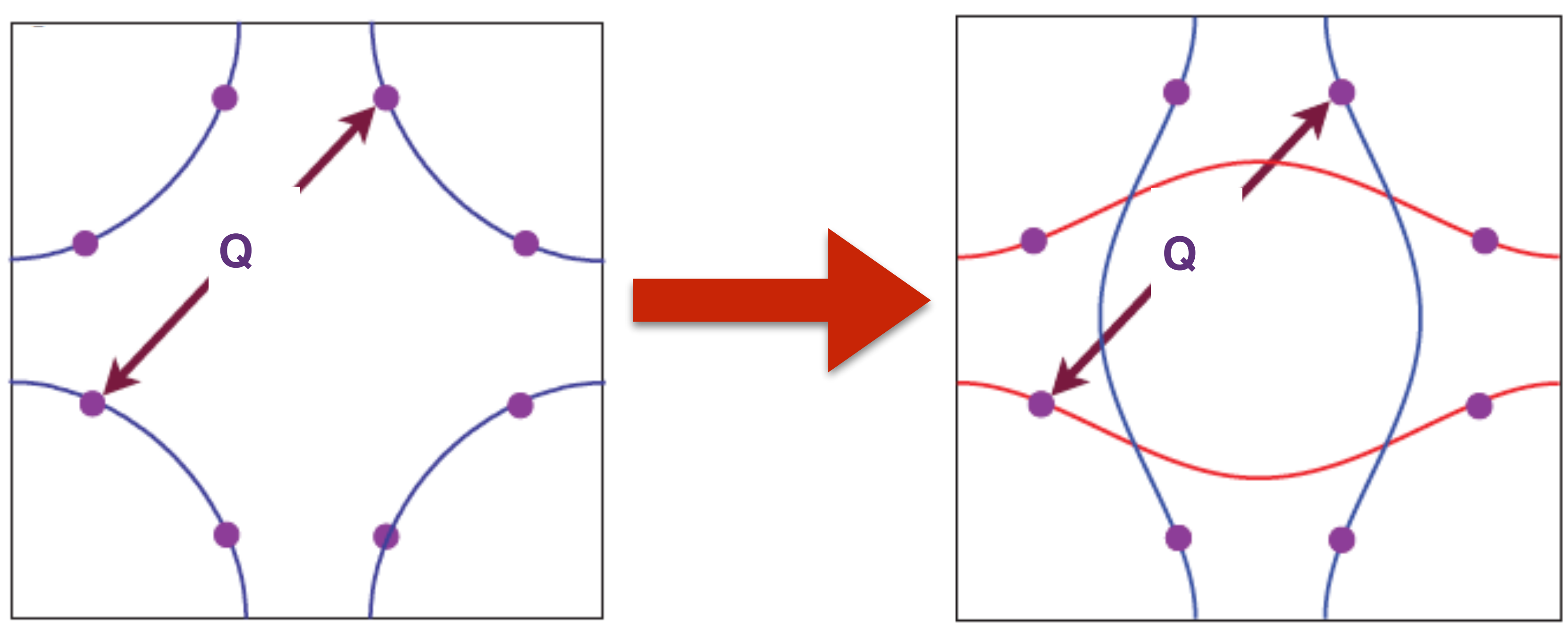
Abanov, Chubukov & Schmalian, Adv. in Phys. (2003)
Metlitski & Sachdev, PRB (2010) …

Sign-free Quantum Monte Carlo method

- How to avoid the fermion sign problem?
  - Two electron bands
  - Spin fluct. couple inter-band
- Kramer's symmetry:

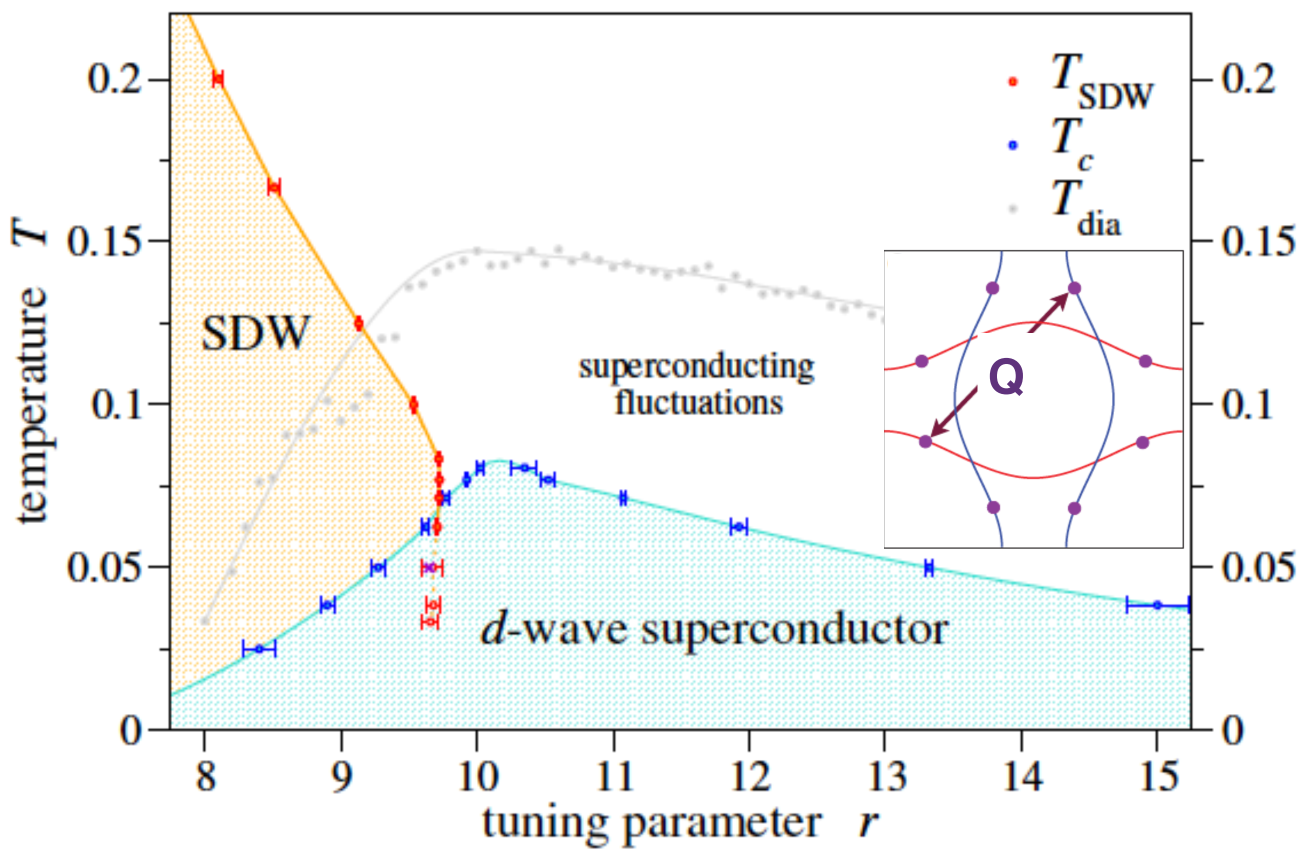
$$\tilde{U} = i\sigma_2 \otimes \tau_3 \mathcal{C}$$

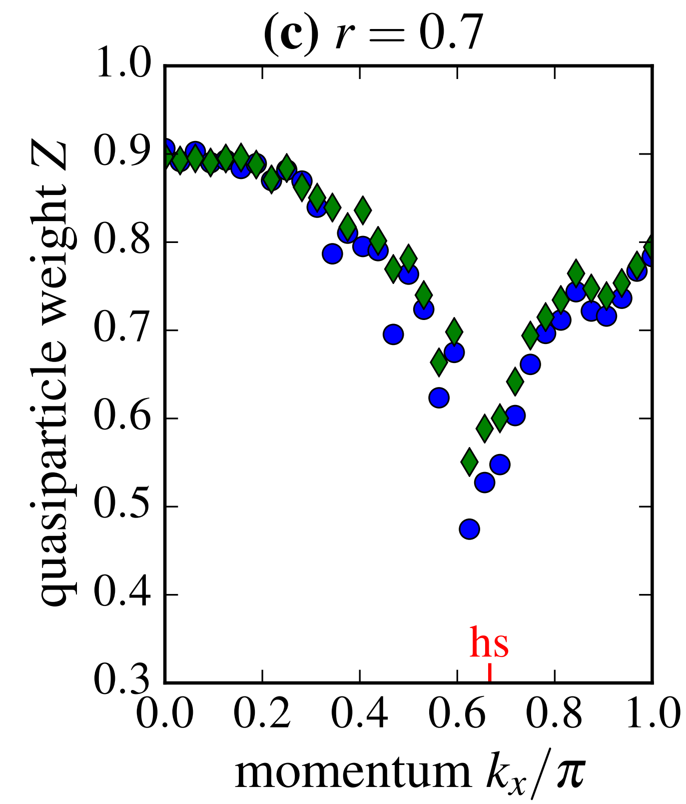
- Hot spots dominate low-energy physics



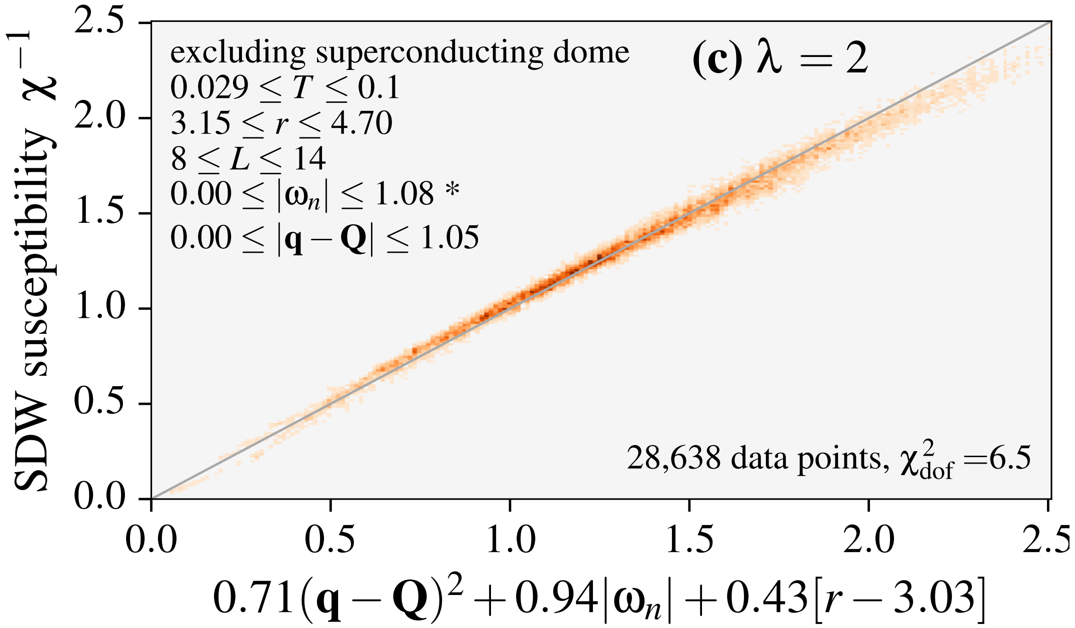
Berg, Metlitski & Sachdev, Science (2012)

Numerical characterization of low-energy properties

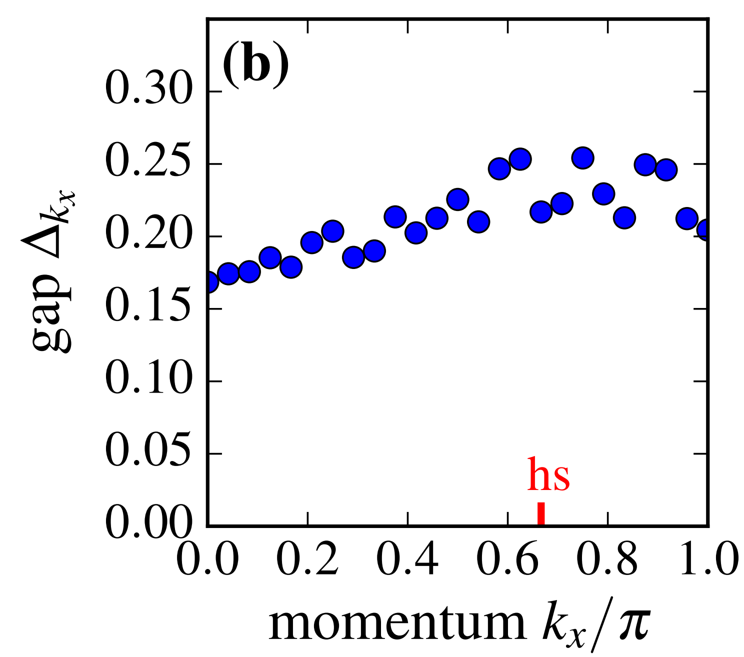




Electrons lose coherence near hot spots



Damping dynamics of spin fluct.



SC gap function **k**-independent

Schattner et al, PRL (2016); Gerlach et al, PRB (2017)

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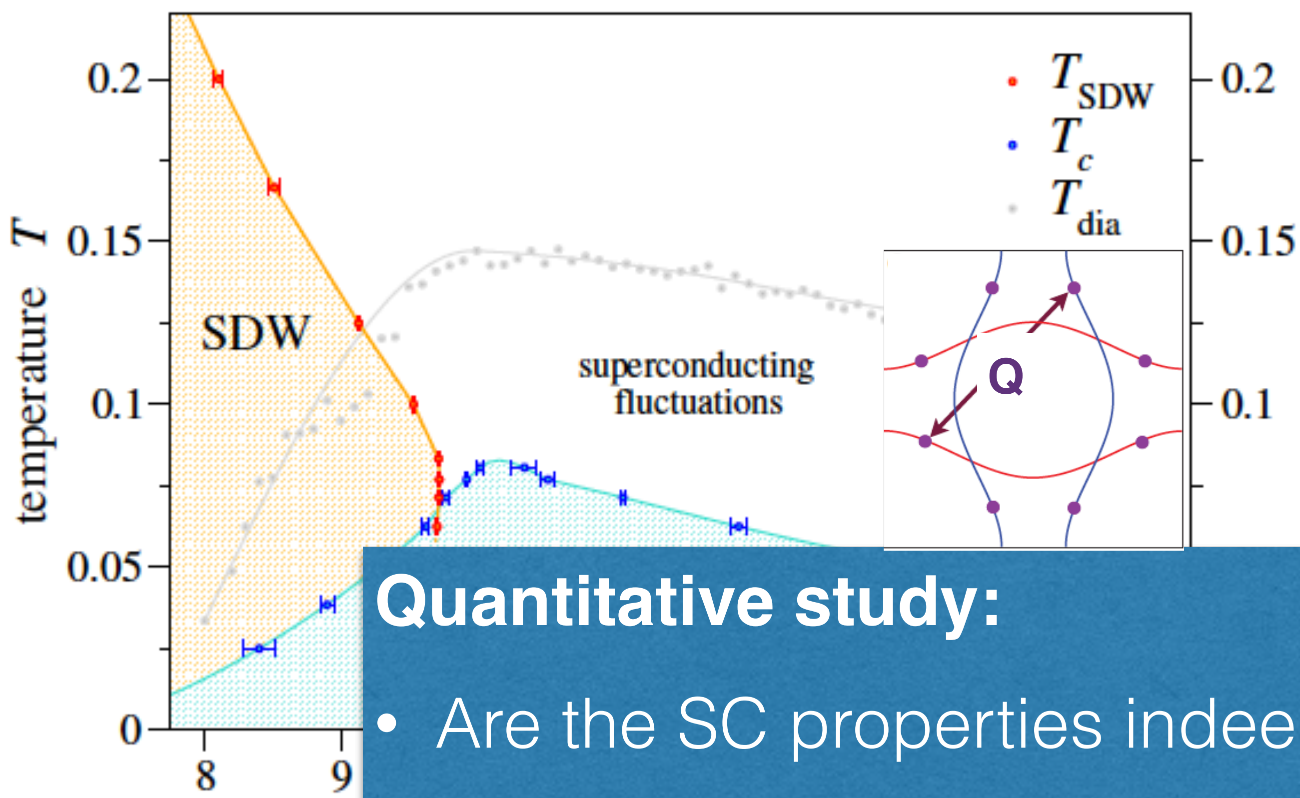
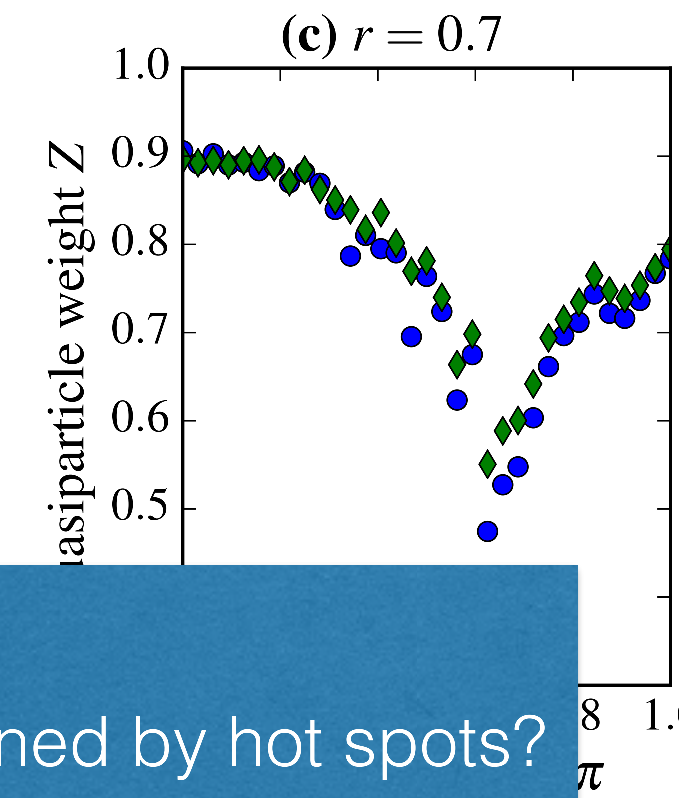
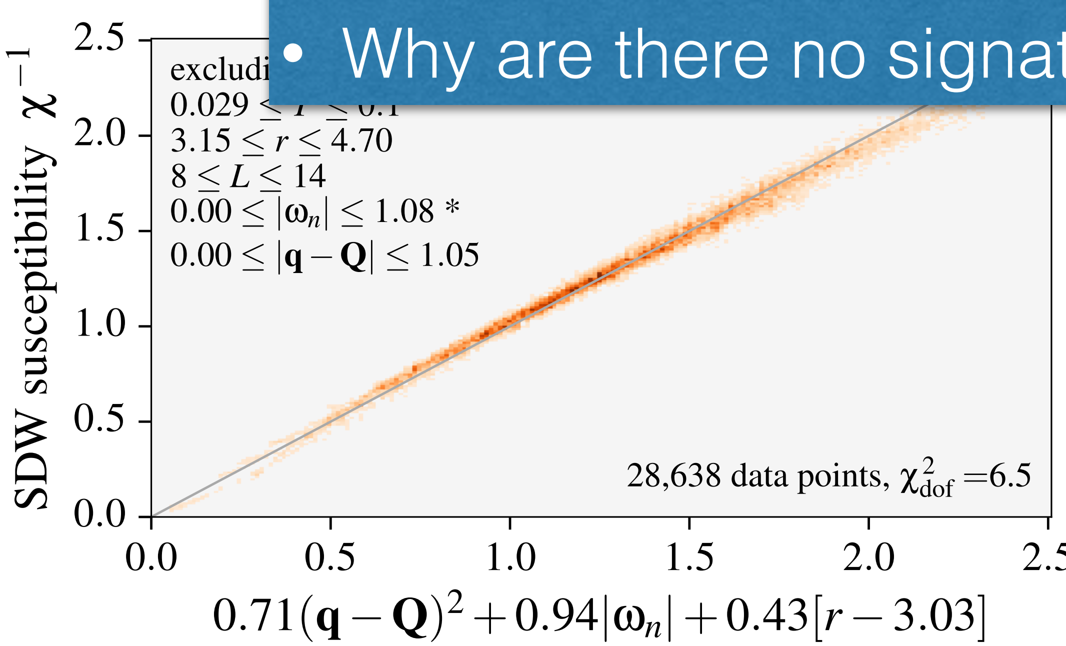




ear hot spots

Quantitative study:

- Are the SC properties indeed governed by hot spots?
- How good is the hot spot Eliashberg approximation?
- Why are there no signatures of CDW?



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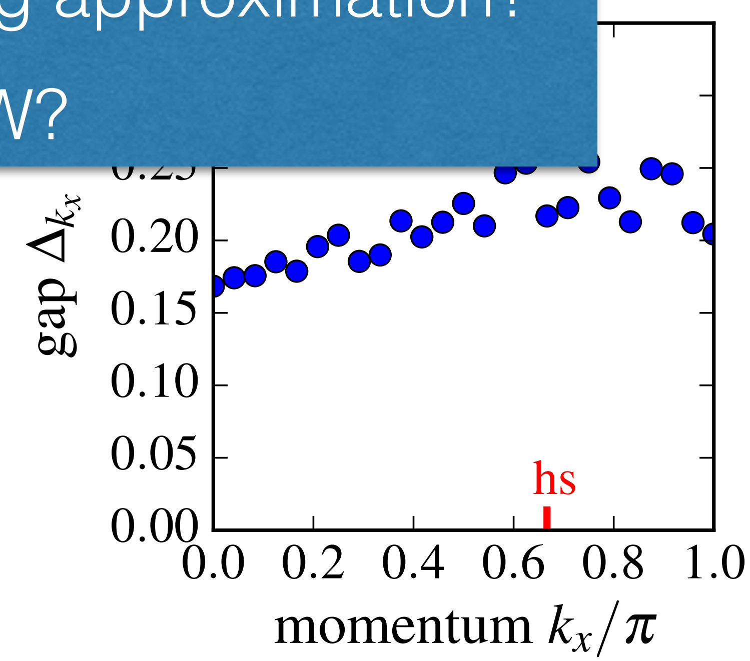
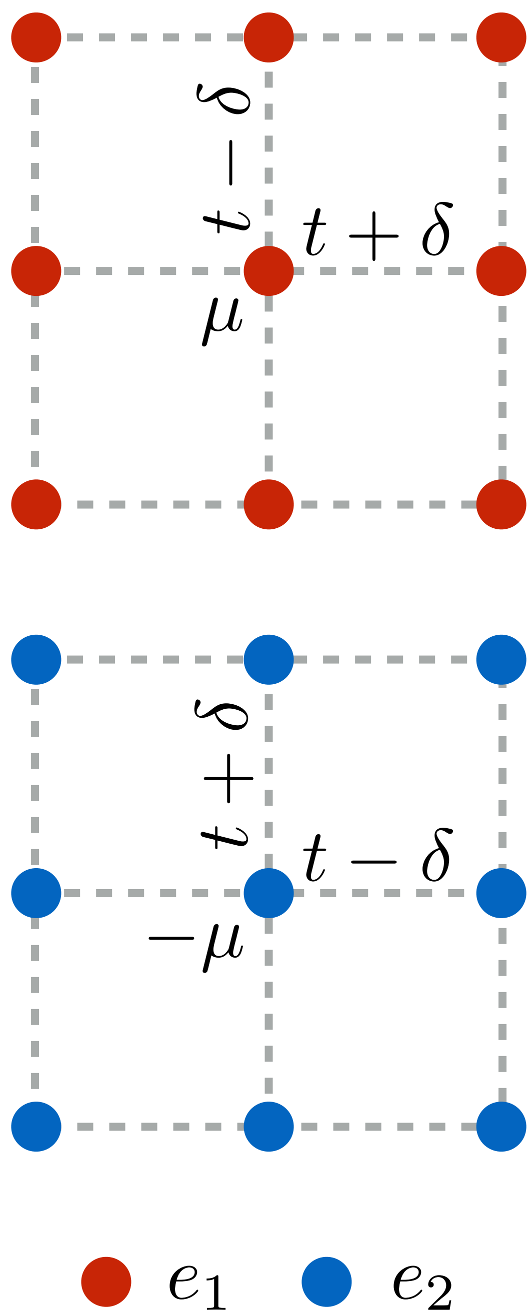


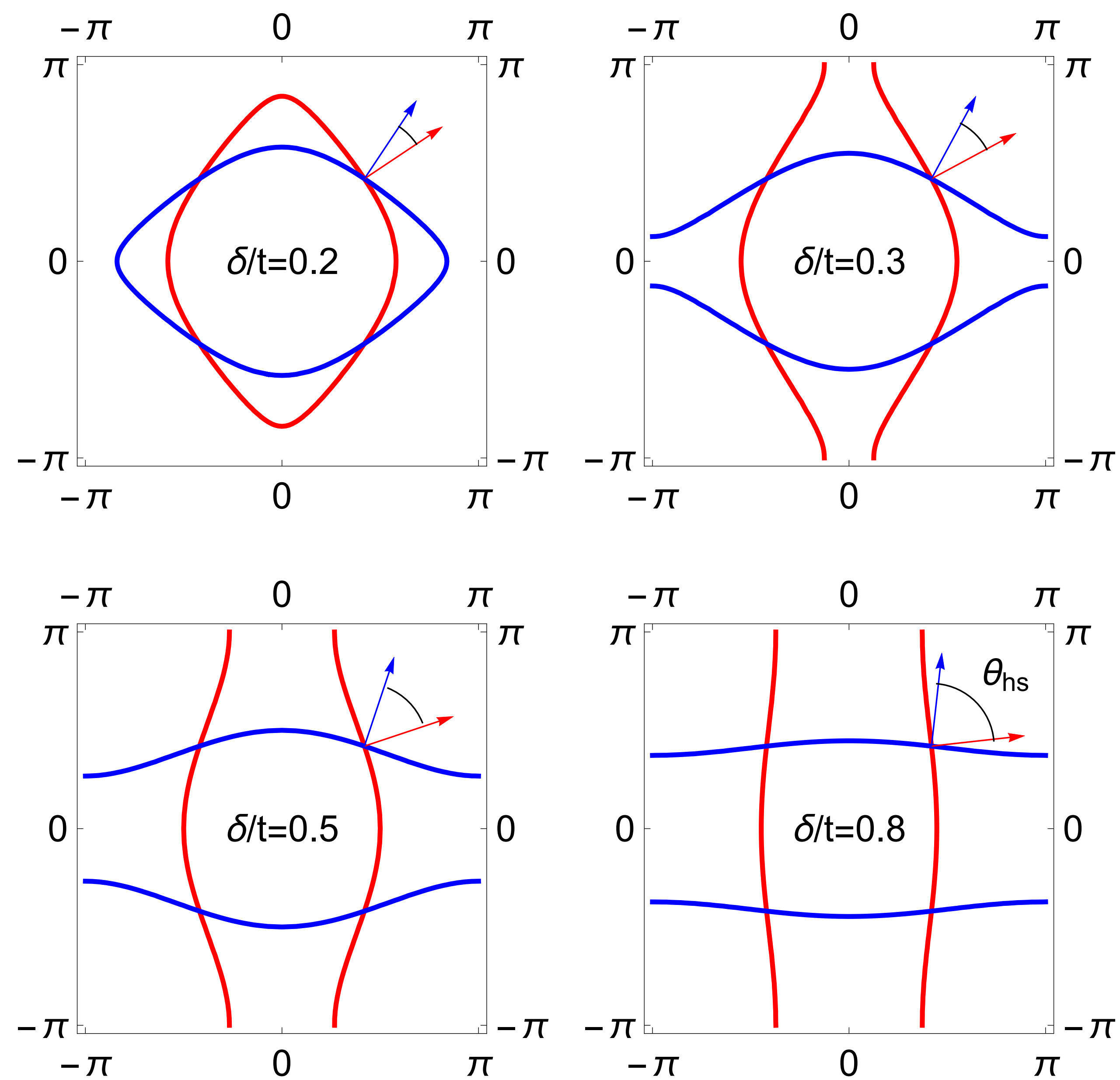
SC gap function **k**-independent

Schattner et al, PRL (2016); Gerlach et al, PRB (2017)

Superconductivity

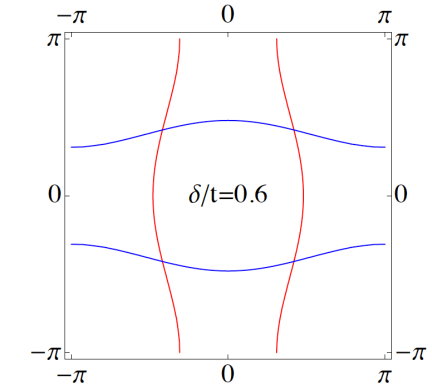
- Study a series of band structures with different δ/t
- Different low-energy properties, while maintaining same bandwidth 8t





Blue band shifted by **Q**; pair of hot spots overlap

Superconductivity



- For each band parameter δ/t :

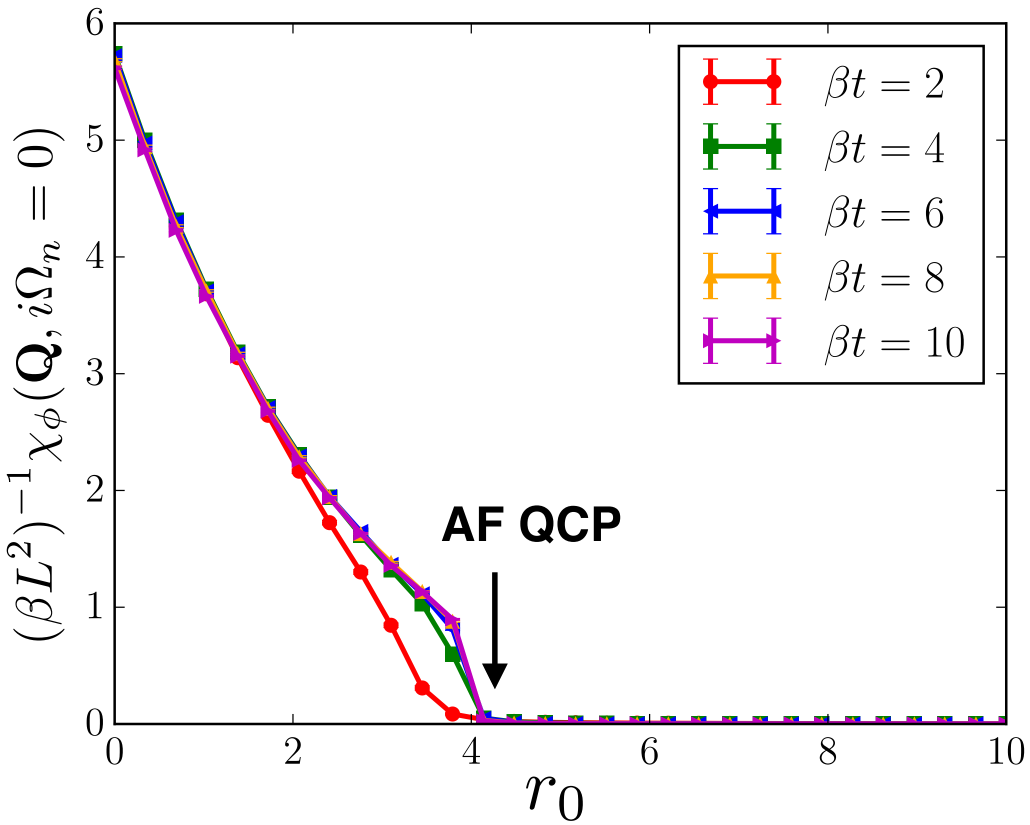
Spin-fermion interaction: $\lambda^2 = 8t$

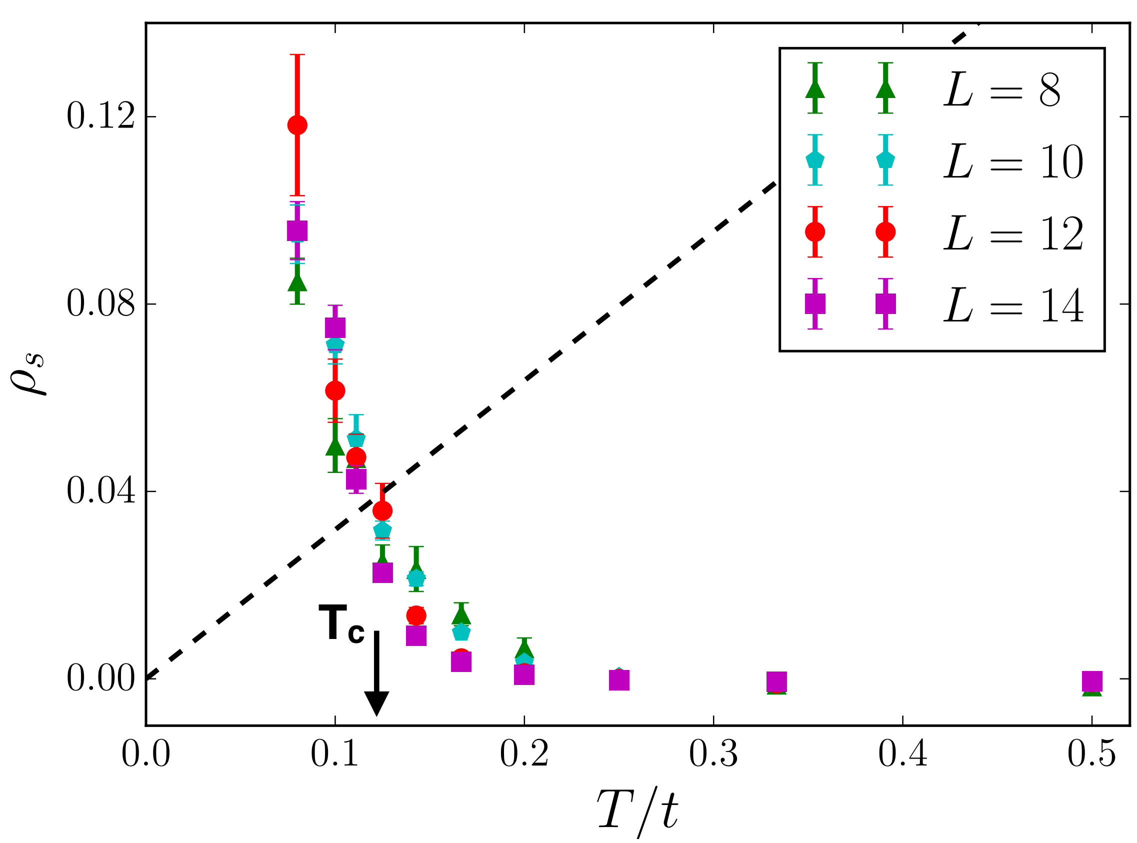
System sizes: $L = 8, 10, 12, 14$

Temperatures: $T \geq 0.04t$

- QMC procedure:
  - Locate AF QCP by varying bare mass r_0 of spin fluct.
  - Obtain T_c via BKT criterion

$$\rho_s(T_c) = \frac{2T_c}{\pi}$$





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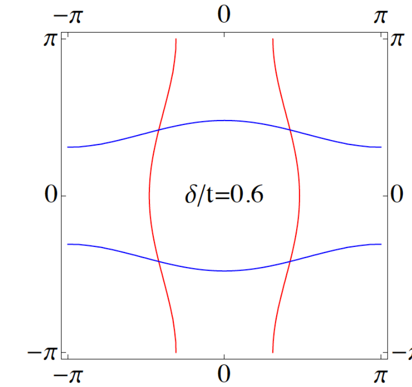

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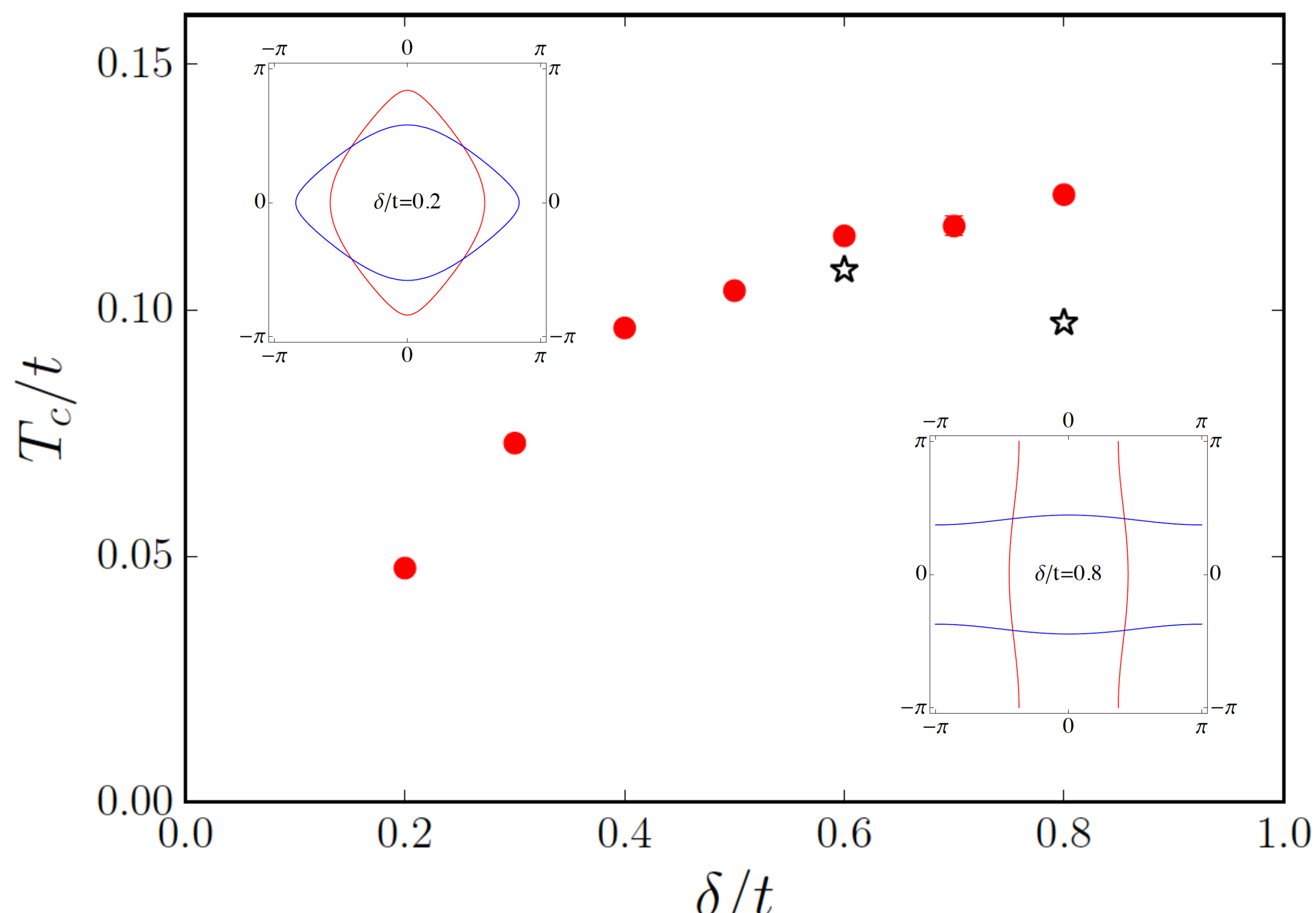
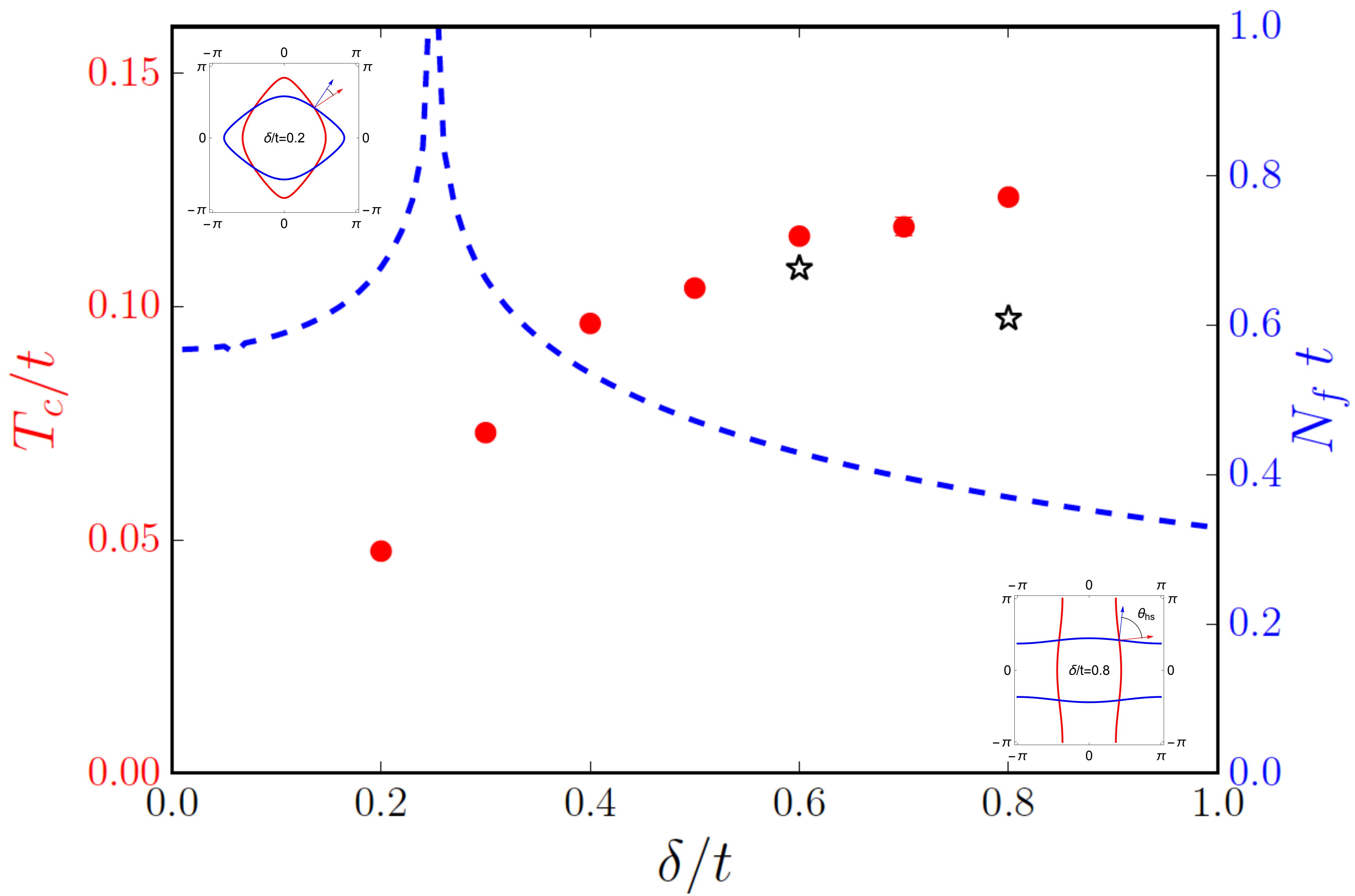


● thermodynamic limit (estimate)

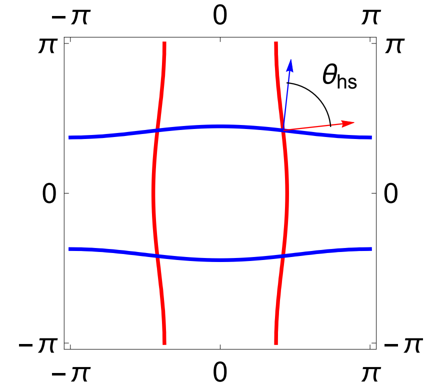
☆ lower bound value

Superconductivity

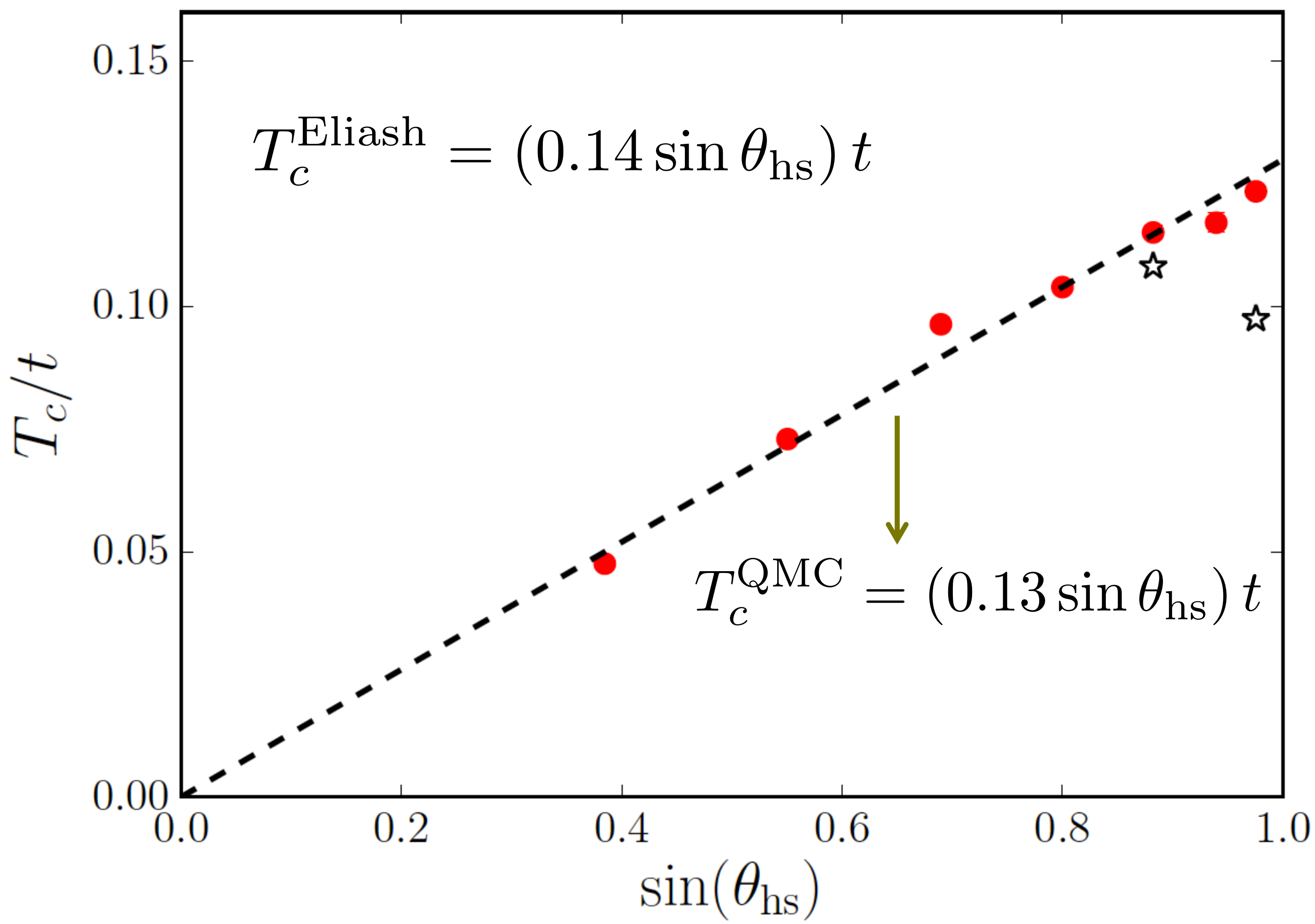
- T_c is not correlated with density of states at the Fermi energy



Superconductivity



- T_c is strongly correlated with the relative angle between Fermi velocities at a pair of hot spots

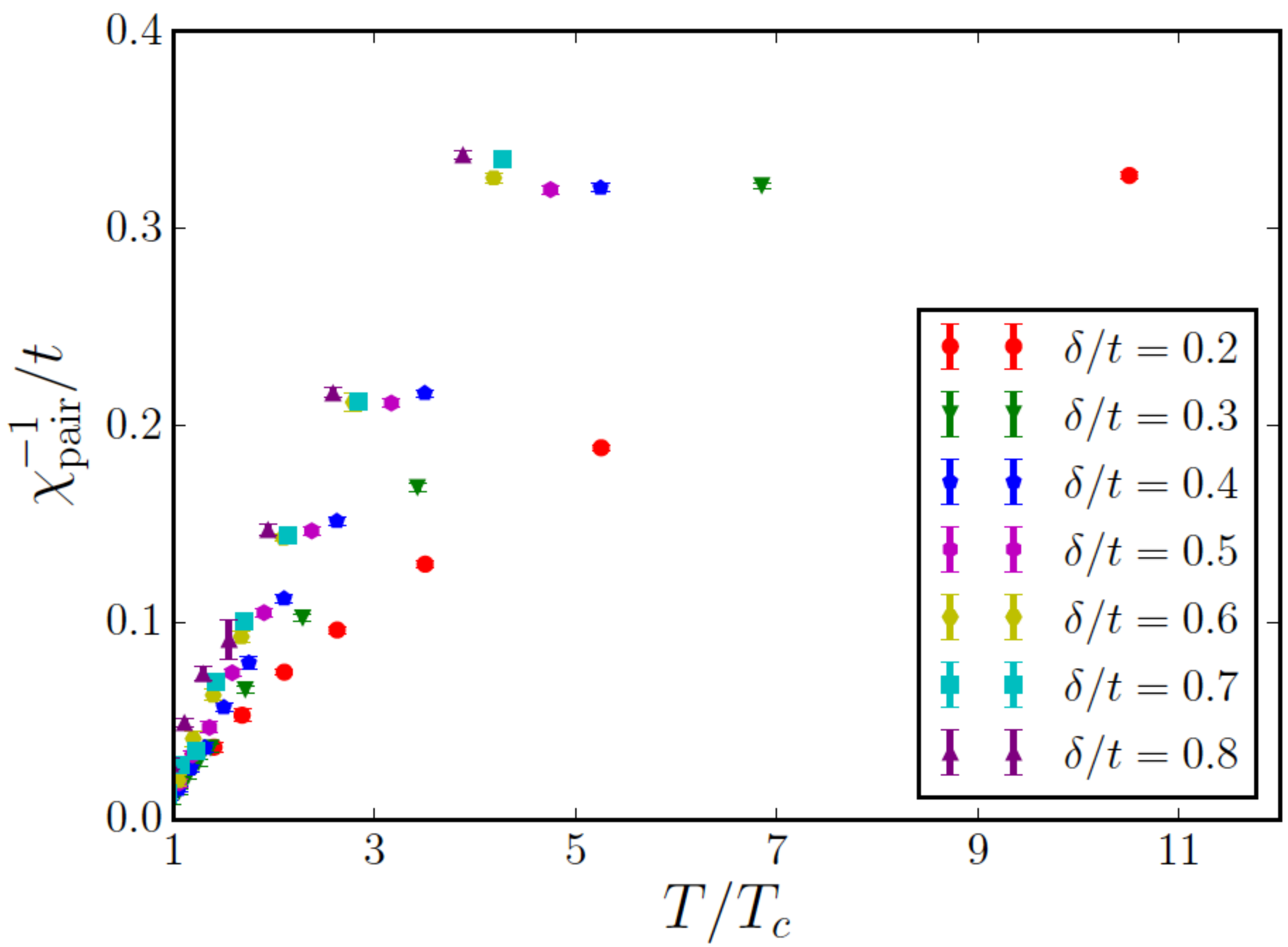


Caveat: Eliashberg T_c does not capture BKT physics

Superconductivity

- Static pair susceptibility:

$$\chi_{\text{pair}} = \int_{\mathbf{r},\tau} \langle \hat{\Gamma}(\mathbf{r},\tau)\hat{\Gamma}^{\dagger}(0,0)\rangle \qquad \hat{\Gamma}(\mathbf{r},\tau) \sim \psi_{\uparrow}(\mathbf{r},\tau)\psi_{\downarrow}(\mathbf{r},\tau)$$



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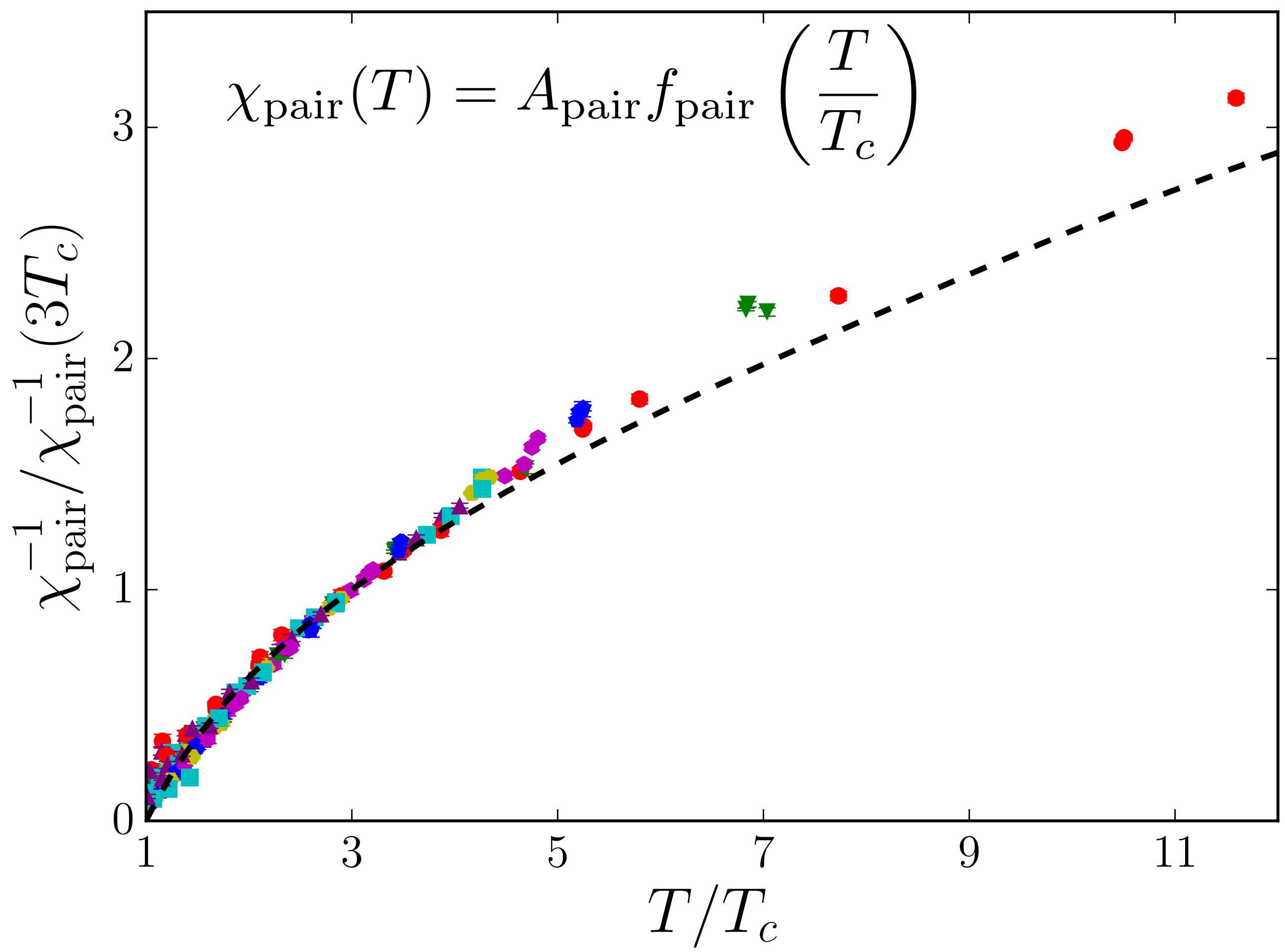
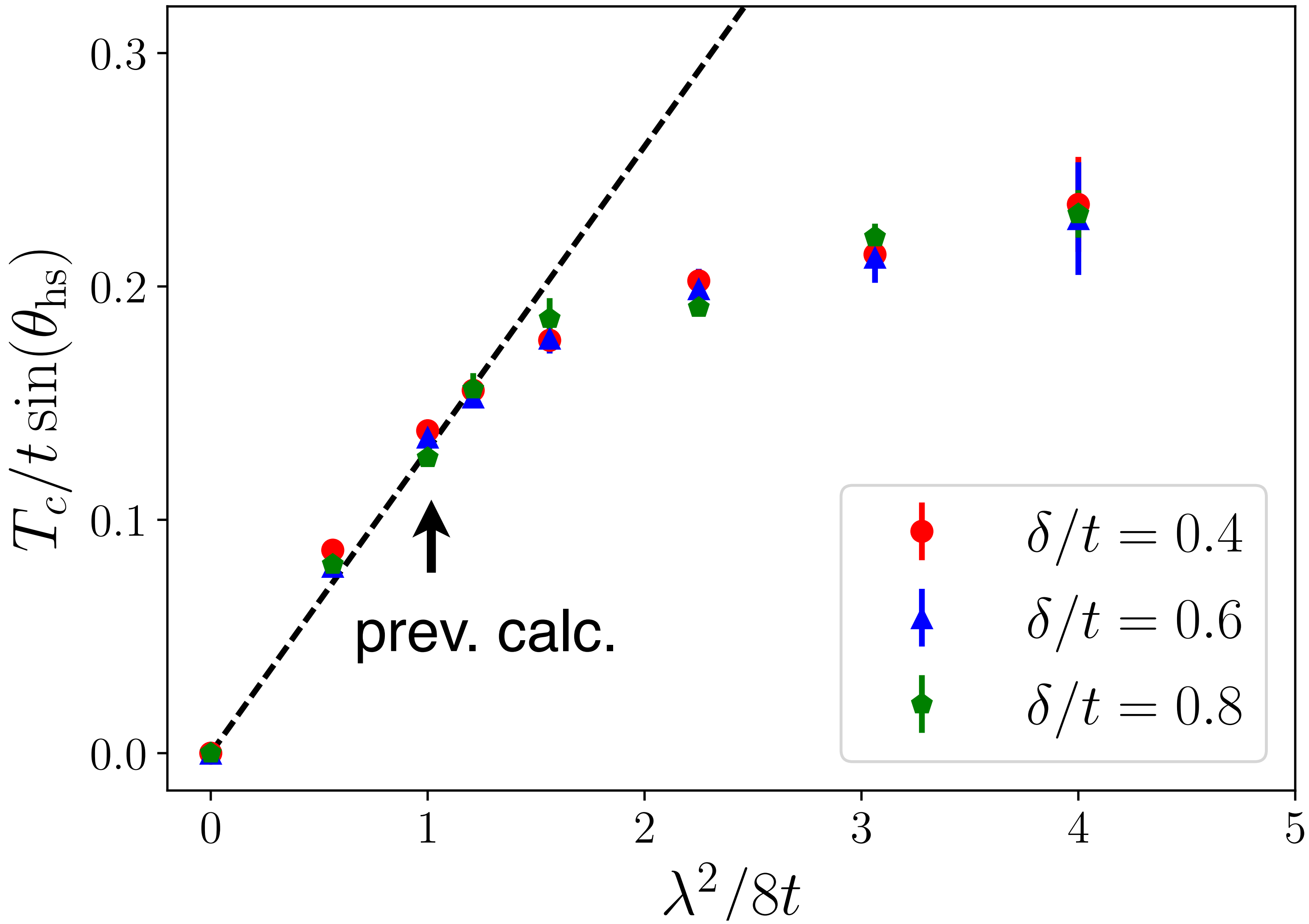


- Scaled susceptibilities collapse onto a ***single universal curve***
- The curve is fitted well by hot spot Eliashberg approximation

Superconductivity

- T_c dependence on the spin-fermion interaction strength: unbounded?

$$S_\lambda = \boxed{\lambda} \int_x \vec{\phi} \exp(i\mathbf{Q}\cdot\mathbf{x}) \cdot \sum_{\alpha\beta} \bar{\psi}_\alpha \vec{\sigma}_{\alpha\beta} \psi_\beta$$



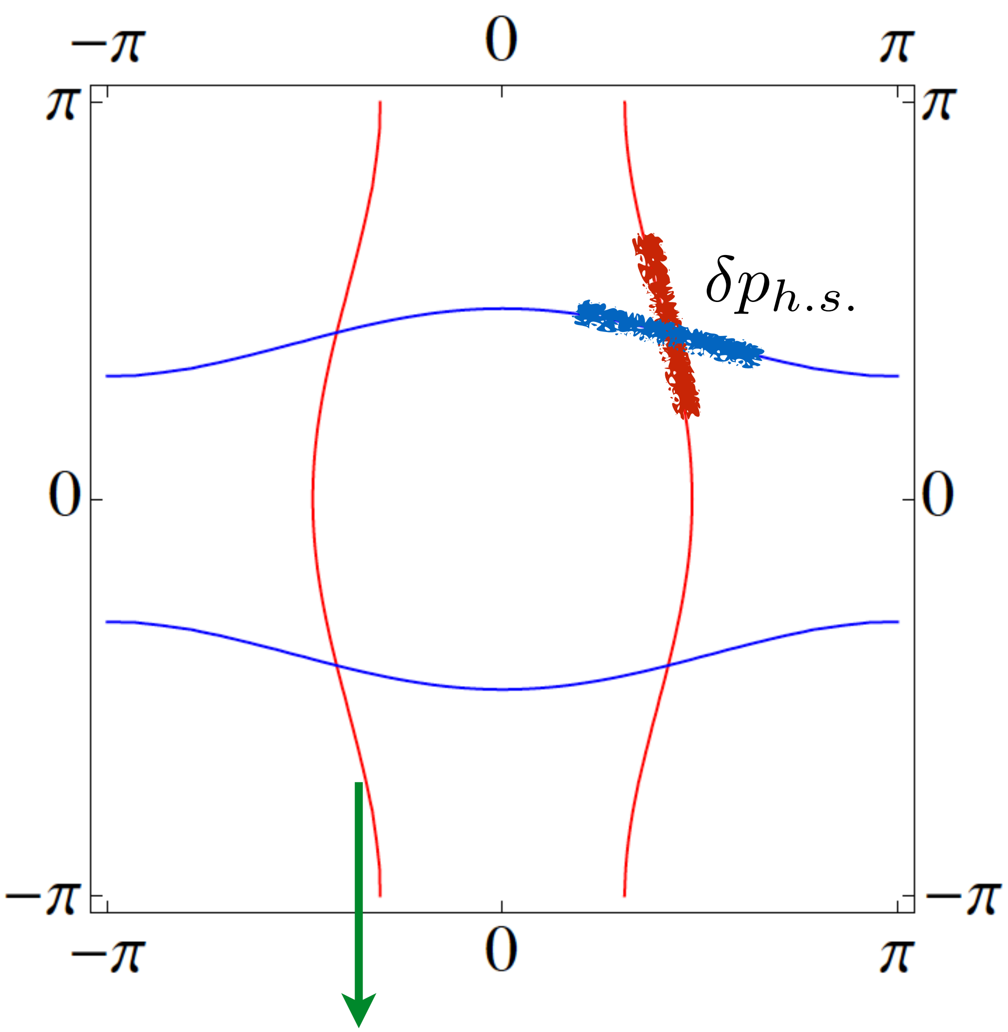
$$T_c^{max} \approx 0.2t$$

Saturation of Tc deviates from linearized hot spot approx. $T_c \propto \lambda^2 \sin\theta_{\rm hs}$

Superconductivity

- Damped spin fluct. propagator:

$$\chi^{-1}(\mathbf{q}, i\Omega_n) = r_0 + (\mathbf{q}-\mathbf{Q})^2 + \boxed{\frac{|\Omega_n|}{\gamma}} \rightarrow (\delta p_{h.s.})^2$$



$$|\mathbf{q}-\mathbf{Q}| \sim p_0$$

$$\frac{\delta p_{h.s.}}{p_0} \sim 1$$

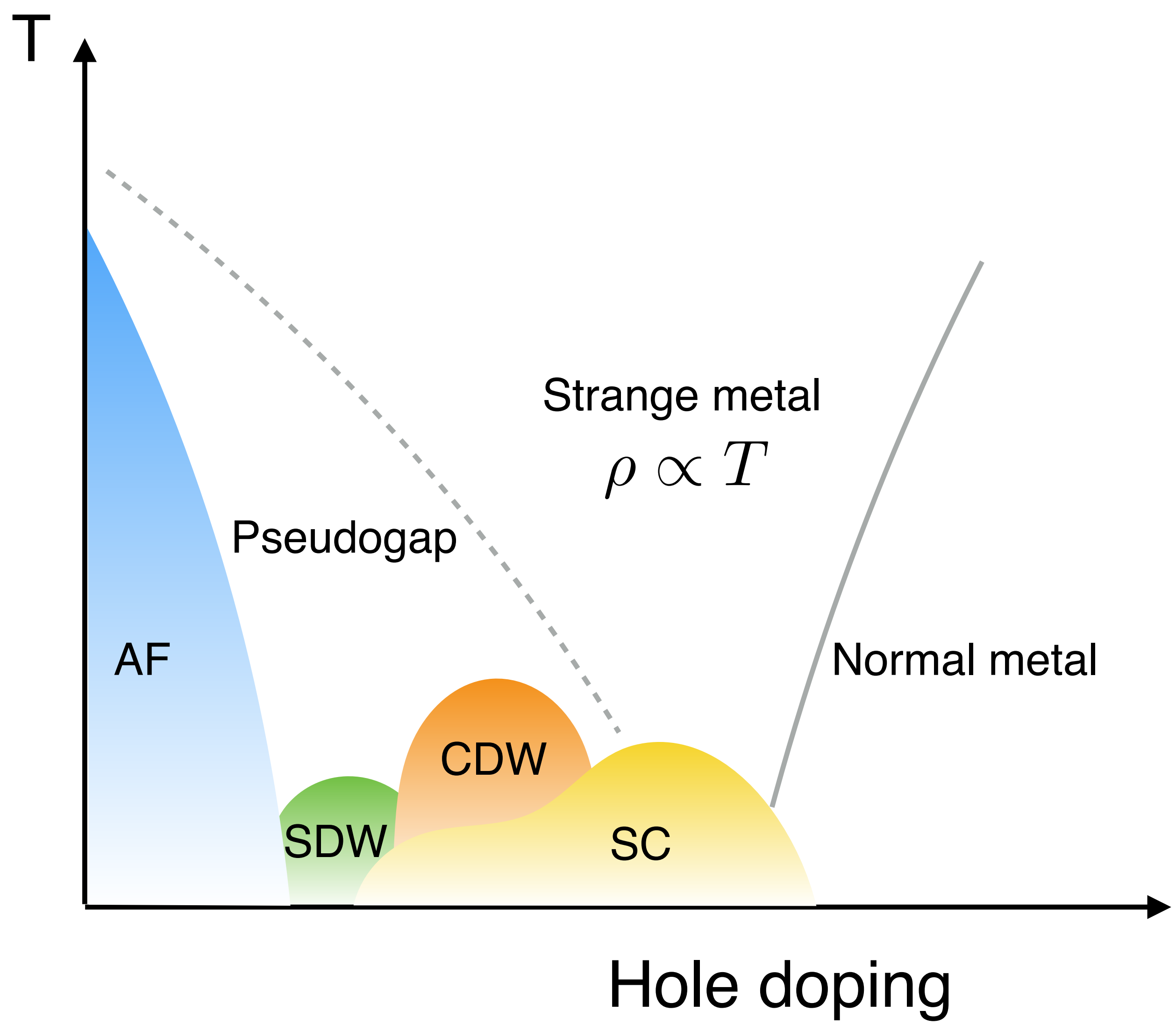
- The whole Fermi surface becomes “hot”
- T_c saturates at crossover from hot-spot dominated to Fermi-surface dominated pairing.

Brief Summary

- Hot spots govern SC properties near AF QCP up to large interactions comparable with fermionic bandwidth
- T_c saturates to a few percent of the bandwidth at the crossover from hot-spot dominated to Fermi-surface dominated pairing
- Despite uncontrolled, Eliashberg approximation shows quantitative agreement with numerical results
  - Why are vertex corrections absent?

Charge Density Wave

- CDW: periodic charge modulations that break translational symmetry
- Observed in the pseudogap region in various hole-doped cuprates
- Competes with SC
- Previous analytical work: CDW can emerge due to spin fluctuations
- Previous QMC: no significant CDW correlations



Experiment:

Chang *et al.*, Nat. Phys. (2012)

Analytics:

Metlitski & Sachdev, PRB (2010)

Wang & Chubukov, PRB (2014)

Numerics:

Schattner *et al.*, PRL (2016)

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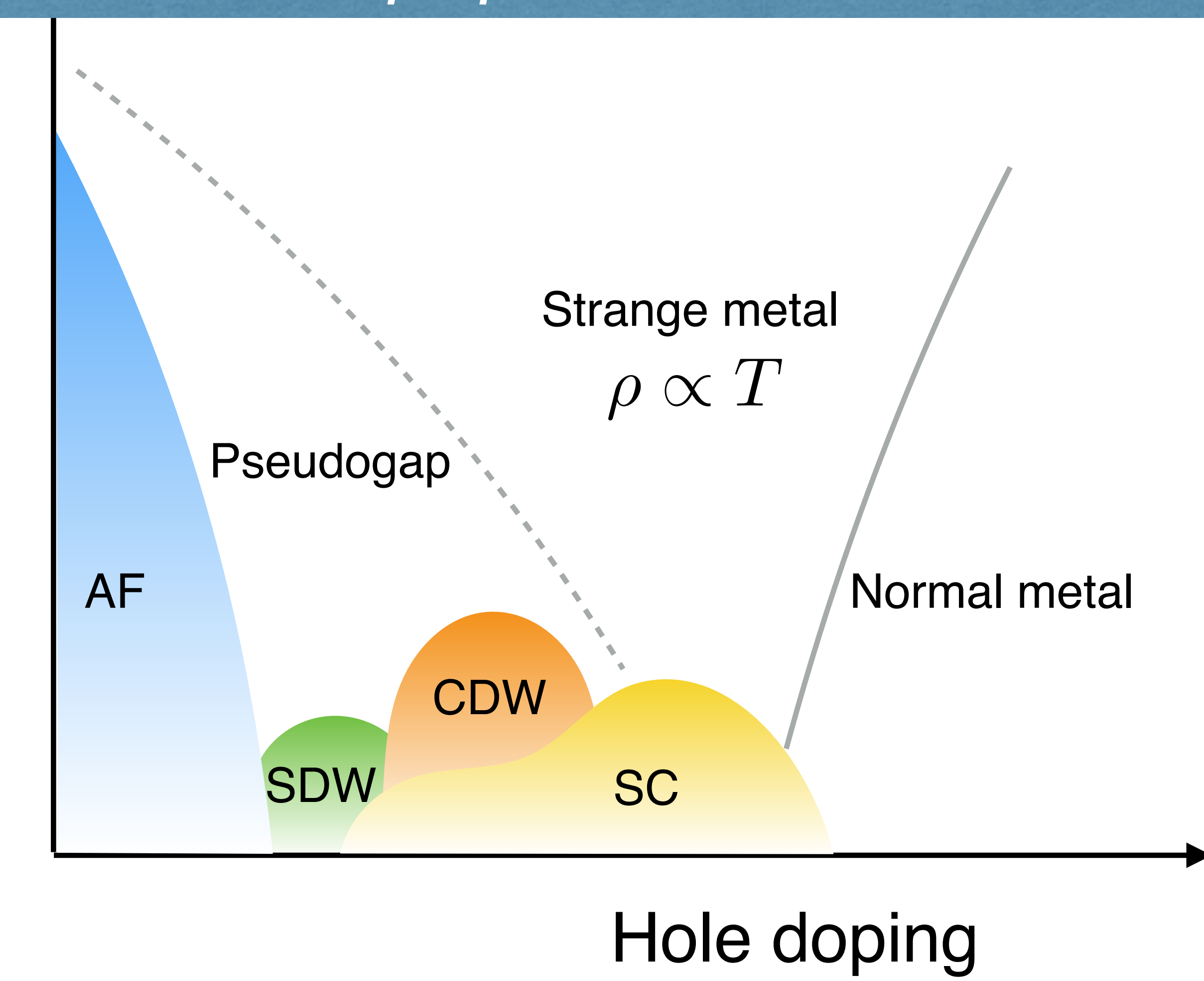
What are the *band properties* to favor CDW in the spin-fermion model?



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- Bipartite lattice at half-filling: exact SU(2) symmetry
    - SC and (π,π) CDW transform like a three-component order parameter
    - Similar symmetries have been studied, e.g., negative-U Hubbard model

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Chakravarty, Laughlin, Morr & Nayak, PRB (2001)

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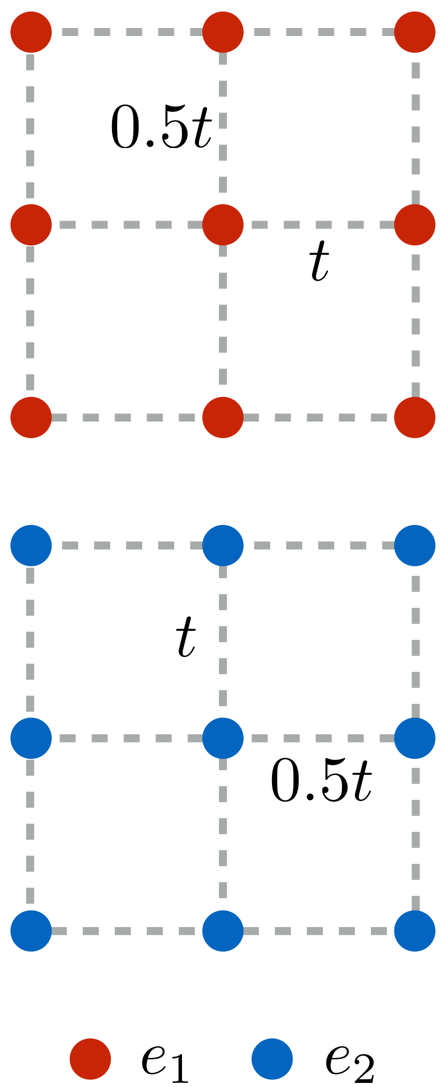

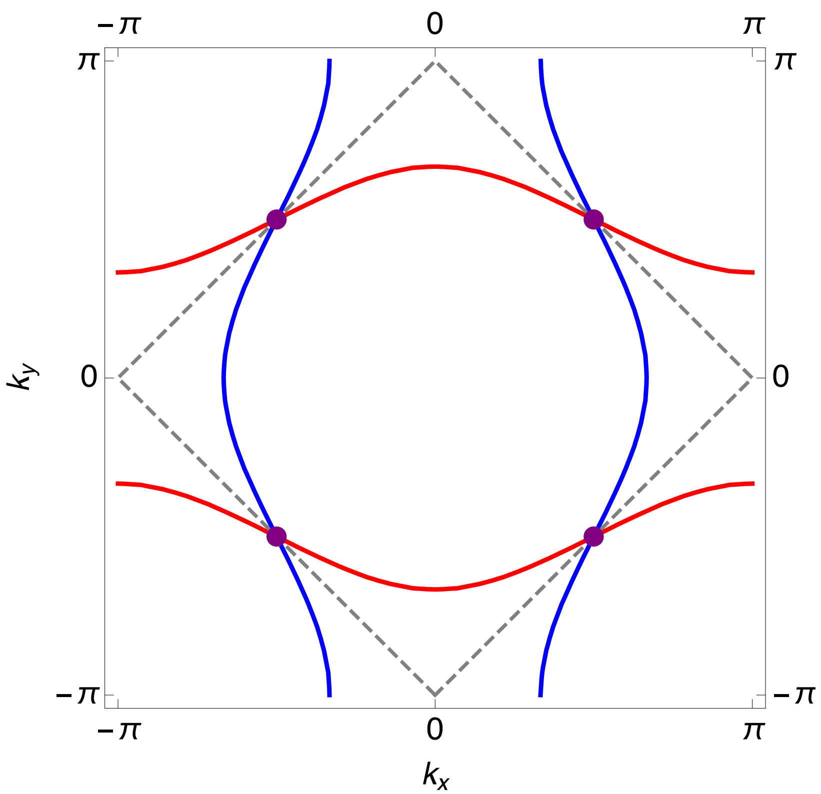

half-filling $\mu = 0$

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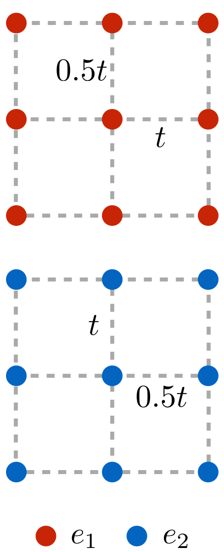

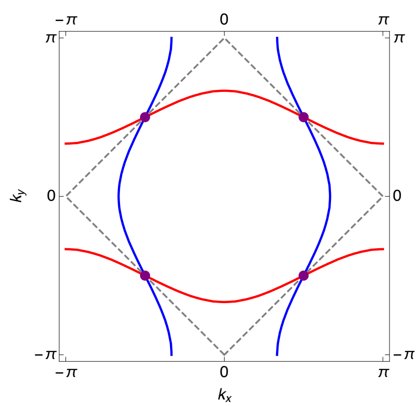

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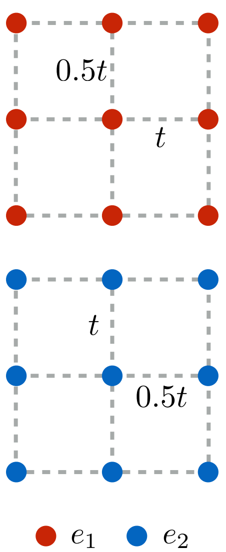

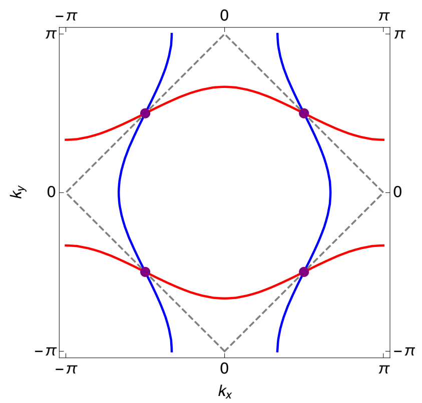

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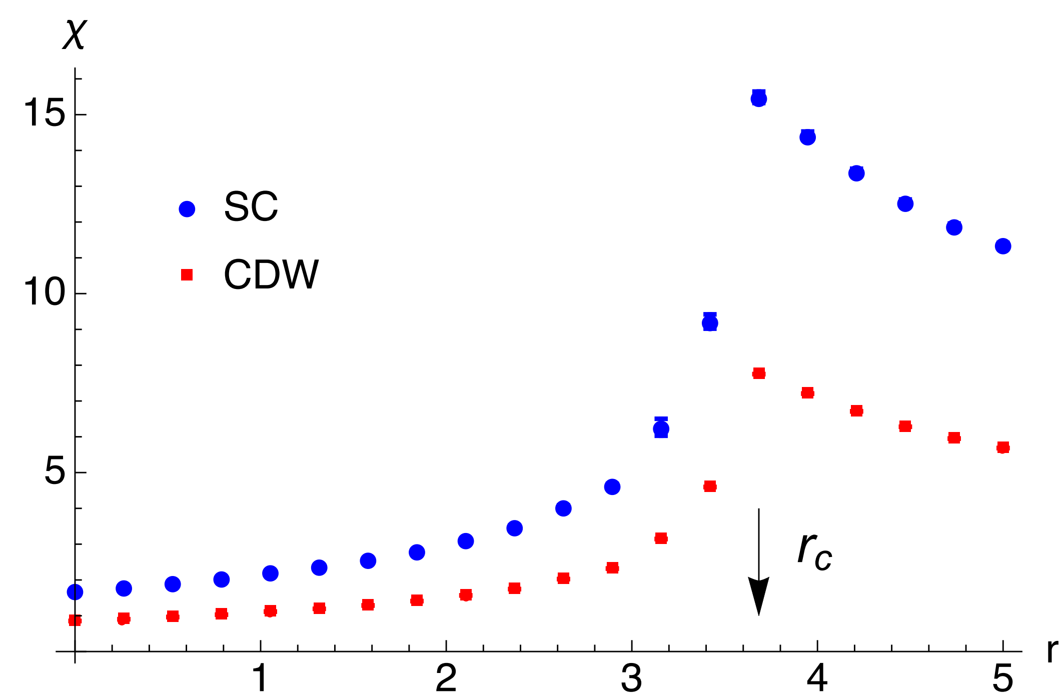
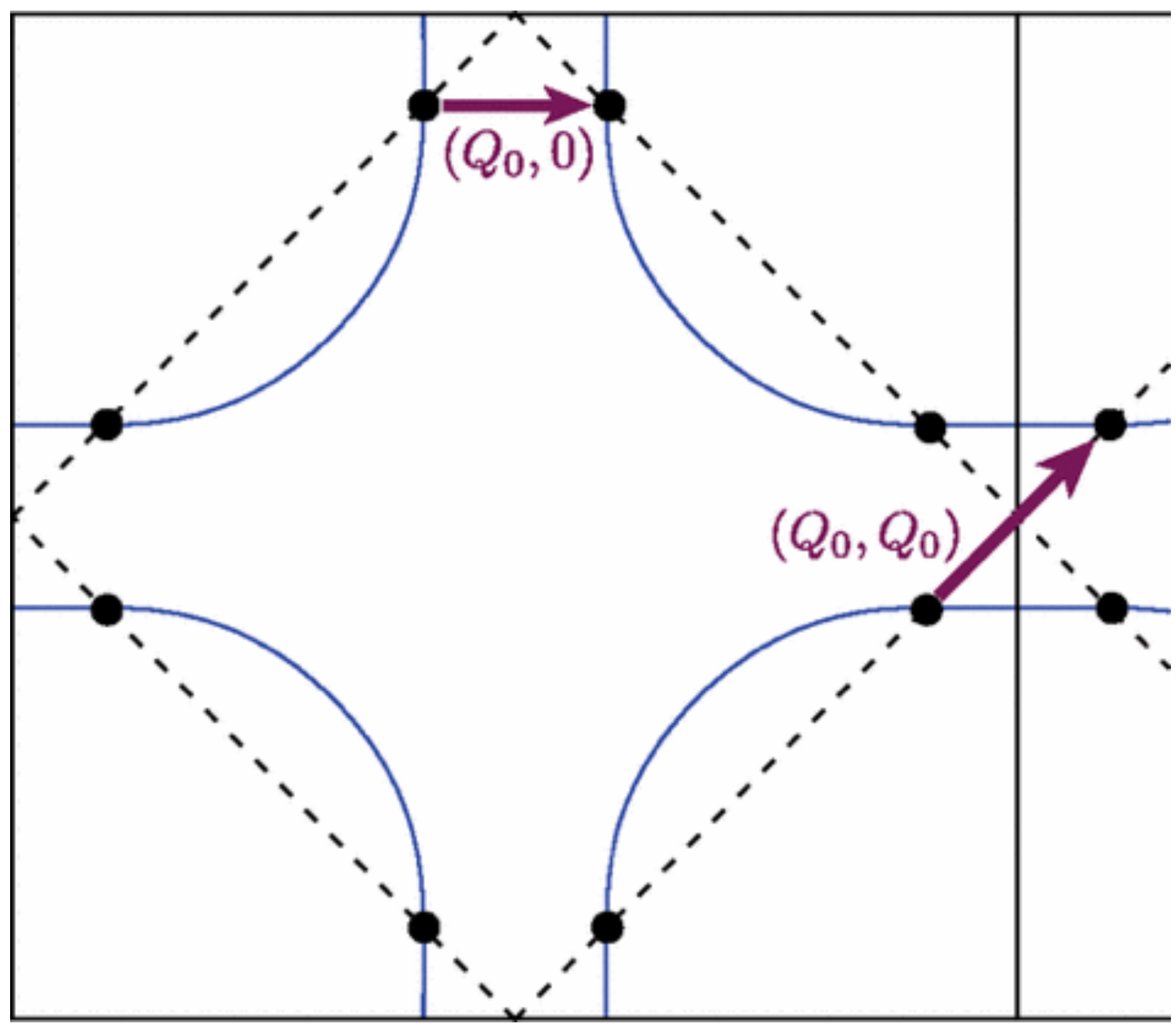
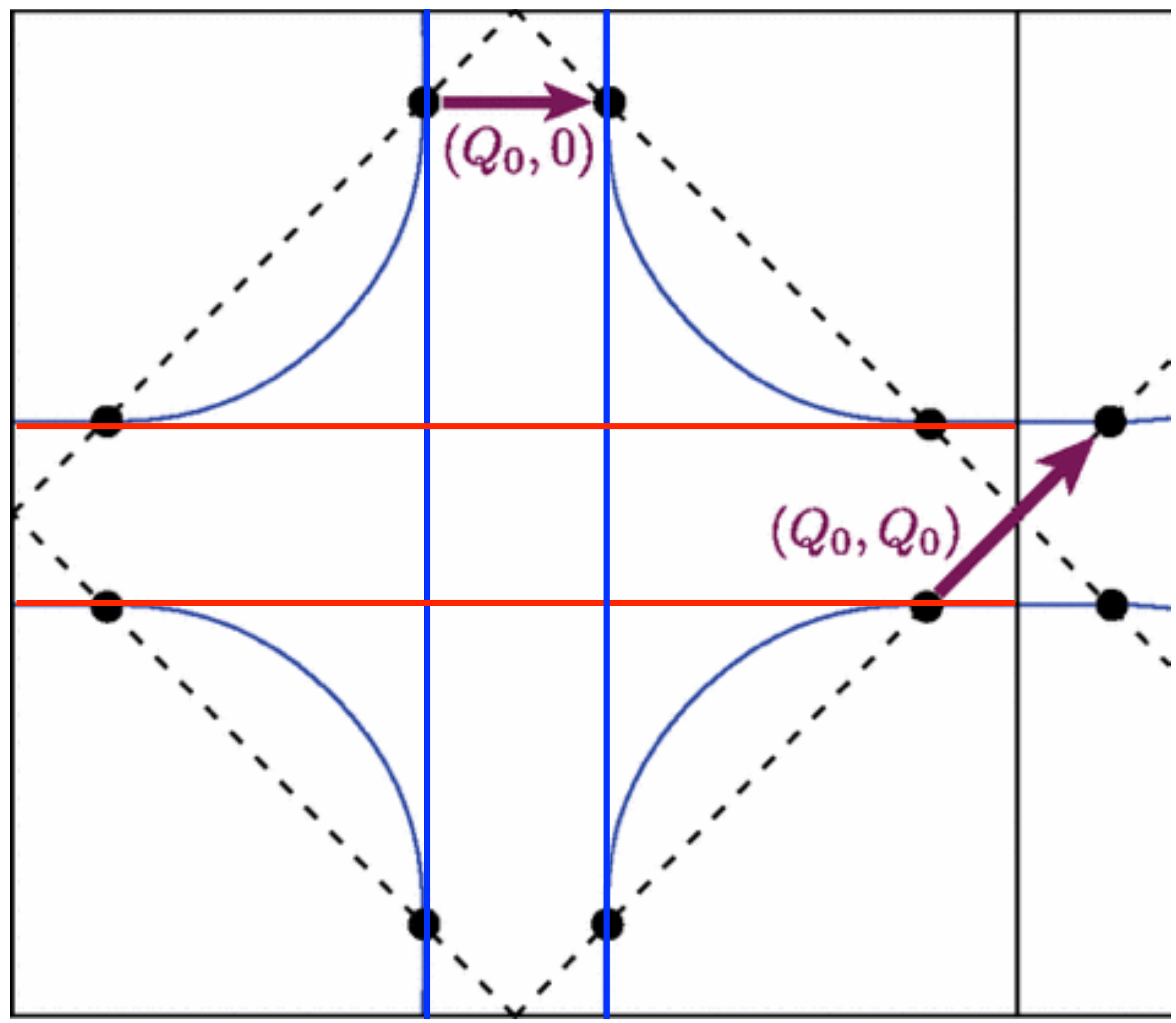


- Can approximate hot spot SU(2) symmetry lead to significant CDW fluctuations?



Sachdev & La Placa, PRL (2013)

- Can approximate hot spot SU(2) symmetry lead to significant CDW fluctuations?
- Consider purely 1D dispersions; exemplify nesting at the antinode



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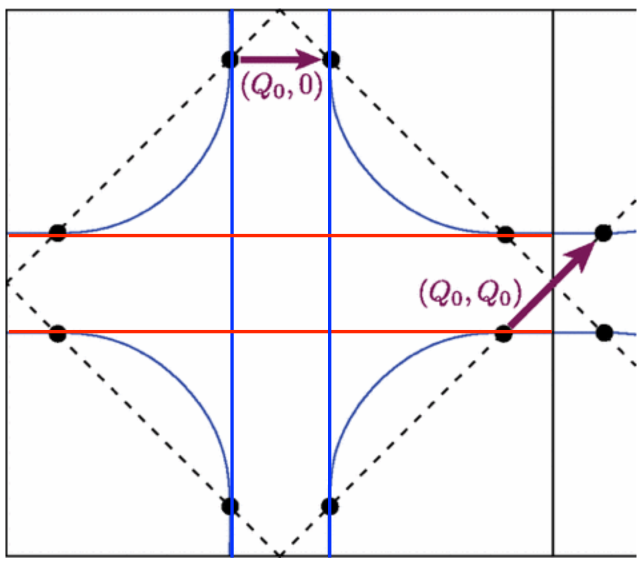

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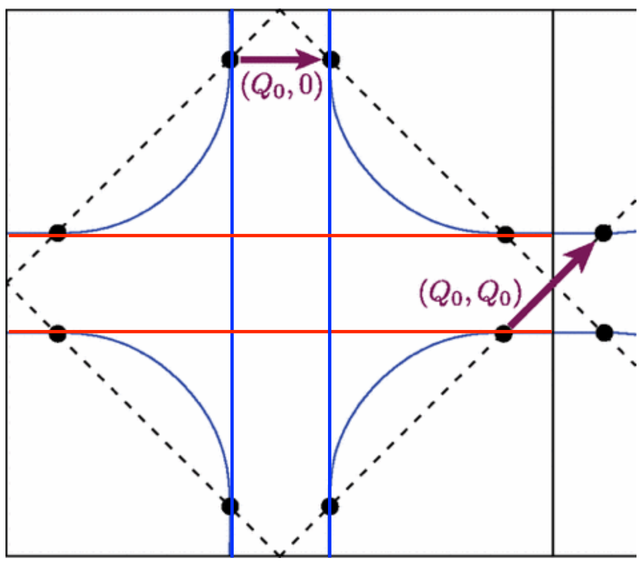

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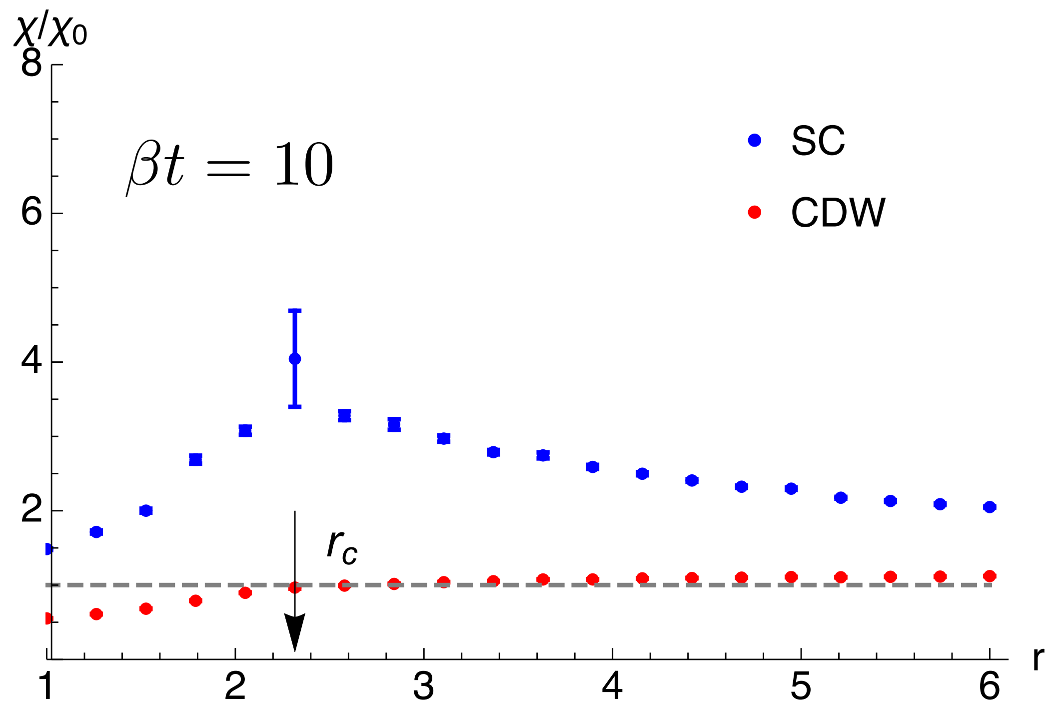
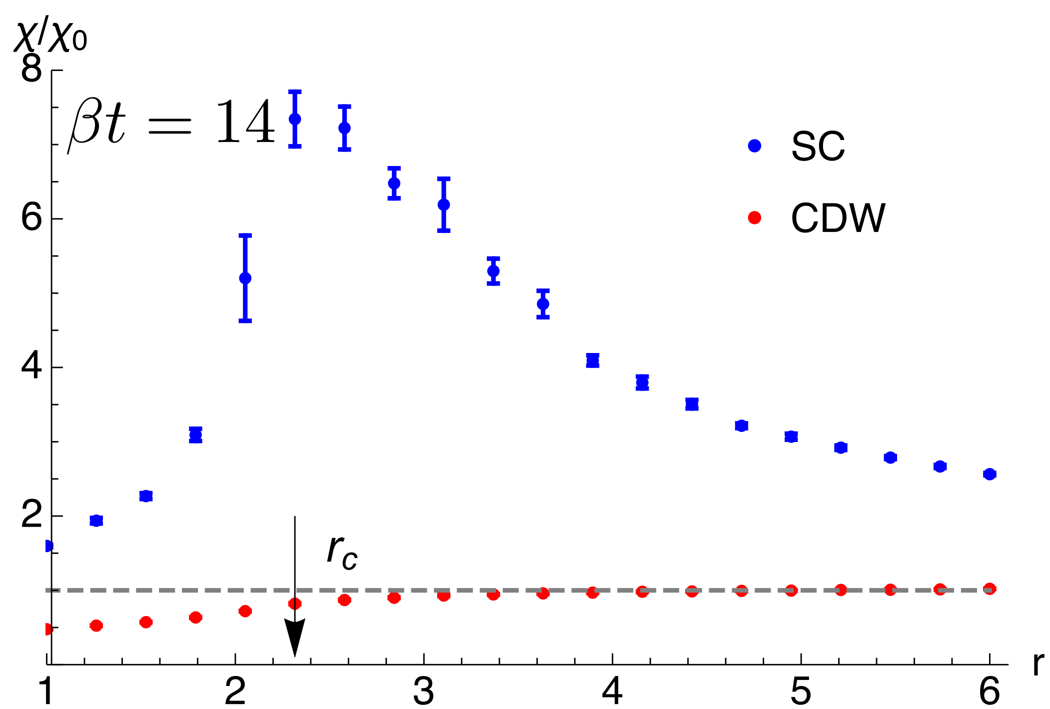
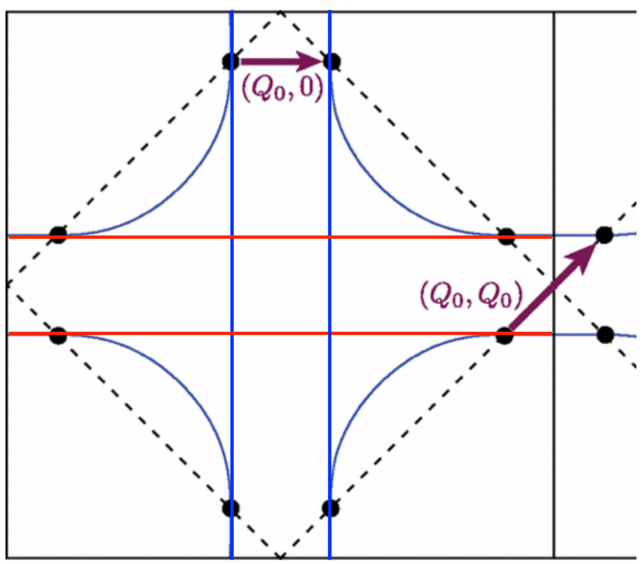




- No near-degeneracy observed
- Strong SC fluctuations suppress CDW

- Can approximate hot spot SU(2) symmetry lead to significant CDW fluctuations?
- Consider purely 1D dispersions; exemplify nesting at the antinode
- Axial versus diagonal CDW?



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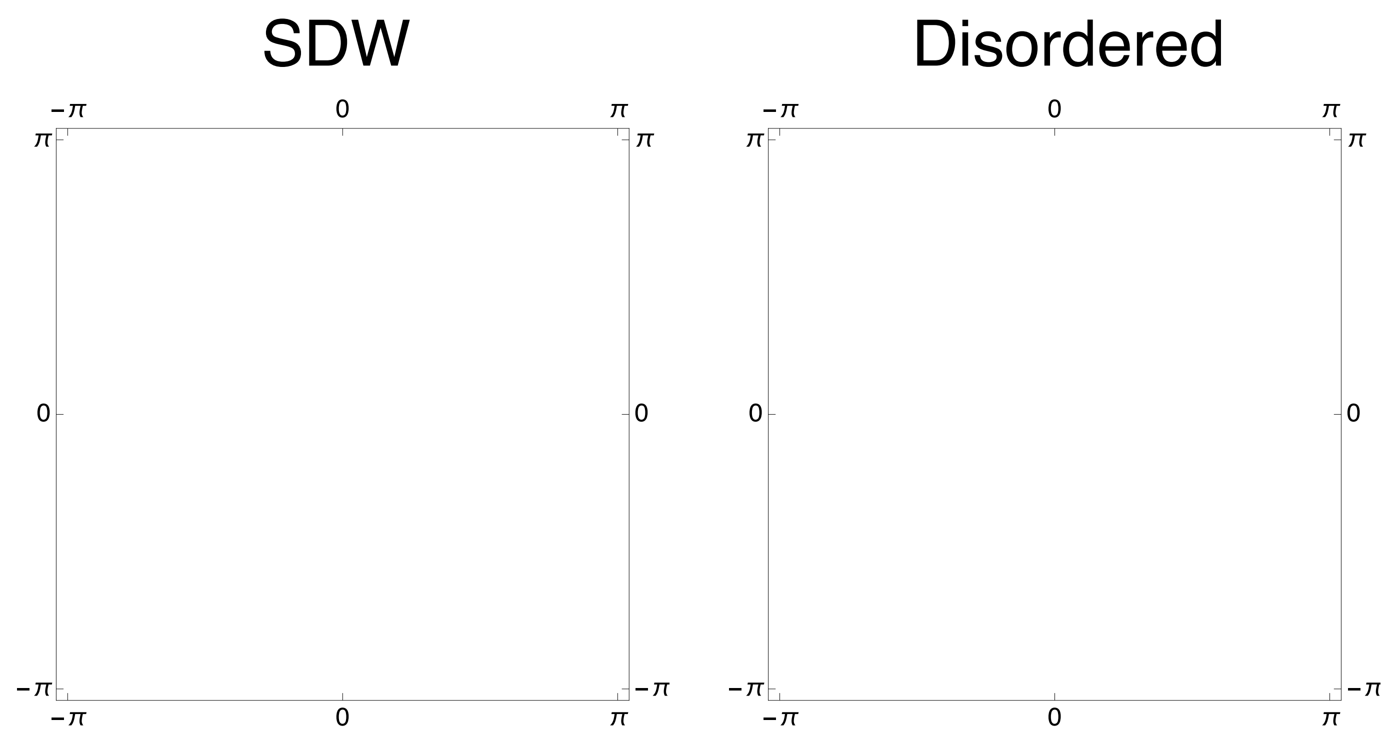

- Shift of CDW wave-vector across magnetic phase transition
  - Fermi surface reconstruction
  - Competition between SC and diagonal CDW

<u>Some other discussions on axial CDW:</u>
Wang & Chubukov, PRB (2014)
Chowdhury & Sachdev, arXiv:1501.00002
…

Summary

- Hot spots govern SC properties near AF QCP up to large interactions comparable with fermionic bandwidth
- T_c saturates to a few percent of the bandwidth at the crossover from hot-spot dominated to Fermi-surface dominated pairing
- CDW is delicate to the fine tuning of Fermi surface properties beyond hot spots
- The approximate symmetry from linearized hot spot approx. insufficient to lead to significant CDW correlations